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User's Manual for OZIPM-4 (Ozone Isopleth Plotting with Optional Mechanisms). Volume 1

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This document describes each of the options in the OZIPM4 program and how to develop the input file needed to run the program.

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VOLUME 1

OFFICE OF AIR QUALITY PLANNING AND STANDARDS
U. S. ENVIRONMENTAL PROTECTION AGENCY
RESEARCH TRIANGLE PARK, NC 27711

JULY 1989

DISCLAIMER

This report has been reviewed by the Office of Air Quality Planning and Standards, U. S. Environmental Protection Agency, and approved for publication. Mention of trade names or commercial products is not intended to constitute endorsement or recommendation for use.

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The original OZIPM-4 User's Manual was prepared by Drs. Gary Whitten and Mike Gery and Mr. Henry Hogo of Systems Applications, Inc., and served as a basis for this manual.

PREFACE

This document is one of five related to application of EKMA and the use of OZIPM-4 (Ozone Isopleth Plotting with Optional Mechanisms), the computer program used by EKMA. Listed below are the titles of the five documents and a brief description of each.

"Procedures for Applying City-specific EKMA", EPA-450/4-89-012, July 1989

- Describes the procedures for using the Empirical Kinetic Modeling Approach (EKMA). The major focus is on how to develop needed inputs for OZIPM-4. In addition this document describes how to determine a control target once OZIPM-4 has been run.

"A PC Based System for Generating EKMA Input Files", EPA-450/4-88-016, November 1988

- Describes a program that creates EKMA input files using a menu driven program. This sofware is only available for an IBM-PC or compatible machine. Files built using this system can be uploaded to a mainframe computer.

"User's Manual for OZIPM-4 (Ozone Isopleth Plotting with Optional Mechanisms)-Volume 1", EPA-450/4-89-009a, July 1989

- Describes the conceptual basis behind OZIPM-4. It describes the chemical mechanism, Carbon Bond 4, and each of the options available in OZIPM-4. Formats for each of the options are outlined so that a user can create input files using any text editor.

"User's Manual for OZIPM-4 (Ozone Isopleth Plotting with Optional Mechanisms)-Volume 2: Computer Code", EPA-450/4-89-009b, July 1989

- Describes modifications to the computer code that are necessary in order to use OZIPM-4 on various machines. A complete listing of OZIPM-4 is also found in this publication.

"Consideration of Transported Ozone and Precursors and Their Use in EKMA", EPA-450/4-89-010, July 1989

- Recommends procedures for considering transported ozone and precursors in the design of State Implementation Plans to meet national ambient air quality standards for ozone. A computerized (PC) system for determining whether an ozone exceedance is due to overwhelming transport is described. This document is necessary, only if an area is suspected of experiencing overwhelming transport of ozone or ozone precursors.

EKMA may be used in several ways: (1) as a means for helping to focus more resource-intensive photochemical grid modeling analyses on strategies most likely to be successful in demonstrating attainment; (2) as a procedure to assist in making comparisons between VOC and NOx controls; (3) in non-SIP applications, such as in helping to make national policy evaluations assessing cost/benefits associated with various alternatives and (4) for preparation of control estimates consistent with limitations/provisions identified in Clean Air Act Amendments.

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1.0 OVERVIEW

1.1 BACKGROUND AND PURPOSE

This report describes the OZIPM-4 model including system structures, computer code, input files, information needed to build the input files and output options.

EKMA was developed as a procedure for relating concentrations of photochemically formed ozone to levels of organic compounds and oxides of nitrogen (EPA, 1977); it utilizes a set of ozone isopleths that depict maximum afternoon concentrations of ozone as a function of the following parameters:

> Morning concentrations of nonmethane organic compounds (NMOC), oxides of nitrogen (NO_x), and carbon monoxide (CO);
>
> Fresh emissions of volatile organic compounds (VOC's), NO_x, and CO occurring during the day;
>
> Transport of pollutants from upwind sources;
>
> Meteorological conditions;
>
> Reactivity of the NMOC mix; and
>
> Biogenic emissions.

The isopleths are developed through computer simulations of atmospheric photochemical reactions using various assumed levels of NMOC and NO_x concentrations. Fresh emissions of VOC's and NO_x are also varied proportionally with the initial NMOC and NO_x levels. The ozone isopleths are then plotted as an explicit function of initial precursor concentrations and an implicit function of emissions, initial CO concentrations, meteorology, transport, reactivity of the NMOC mix and biogenic emissions. The isopleths are used to compute the percent reduction in NMOC that is needed to lower peak ozone to the concentration

(0.12 ppm) specified in the national ambient air quality standard (NAAQS) for ozone.

A computer program was developed to readily generate the ozone isopleths for EKMA users. This program is called the Ozone Isopleth Plotting Package (OZIPP). Detailed documentation of EKMA and OZIPP is given in EPA (1977); Whitten and Hogo, (1978a); EPA (1981); EPA (1984); and Hogo and Whitten, (1985).

Since its origin, more sophisticated versions of the OZIPP model have been developed. These models are:

> OZIPM--Version 1--a computer routine with the capability of handling different chemical kinetics mechanisms (Whitten and Hogo, 1978b).
>
> OZIPM--Version 2--this version of OZIPM contains some code modifications to the original version so that it can be used easily on different computer systems. This version also has the capability of calculating the needed percent reduction in NMOC without first generating an isopleth (Gipson, 1984).
>
> OZIPM--Version 3--a new mechanism, called the CBM-X, which was recently developed and tested against auto exhaust smog chamber data, has been incorporated into this version. The results of that work are described in Whitten et al. (1985).
>
> OZIPM--Version 4--the current version is an update to OZIPM3. This version requires less computer memory and contains some internal code modifications to correct computer errors associated with OZIPM3. The default chemical mechanism is CBM-4, a condensed version of CBM-X (Whitten and Gery, 1986).

OZIPM-4 is the software currently applied in regulatory applications of EKMA. Volume 1 serves as the User's Manual for OZIPM-4. Section 2 of this volume contains an overall technical description of how OZIPM-4 operates. Section 3 presents a detailed description of the different input and output options available for applications of OZIPM-4. Section 4 provides information on how to select input options when using the CBM-4 chemical mechanism stored in OZIPM-4. Section 5 contains a summary of the options discussed in Sections 3 and 4 and serves as a quick reference guide for the user. Users interested only in running the program can skip to this section. Section 6 contains examples of model runs. These examples demonstrate the use and flexibility of OZIPM-4. Volume 2 contains the computer code listing of OZIPM-4.

Much of the discussion of concepts and model applicability in the original OZIPP manual applies to OZIPM-4. However, in Volume 1, we repeat some of this information for the sake of convenience.

1.2 SCOPE OF USE AND LIMITATIONS

The OZIPM-4 is limited in applicability to ozone problems within, or immediately downwind of, large urban areas, and thus should not be applied to the following situations unless special attention is given to existing limitations and assumptions:

> The rural ozone problem;
>
> Situations in which transported ozone and/or precursors are clearly dominant (i.e., multi-day transport situations);
>
> Cases in which the maximum ozone concentration occurs at night or in the early morning; and
>
> Development of control strategies for single or small groups of emission sources.

The validity of an ozone isopleth diagram generated by OZIPM-4 for a particular city may be affected by the following considerations:

> The kinetic mechanism used to describe the transformations of NMOC and NO_x;
>
> The physical assumptions used to formulate the trajectory model coded into OZIPM-4;
>
> The meteorological data and assumptions used to specify the parameters required to apply OZIPM-4;
>
> The availability and reliability of current ozone data, precursor concentration data, and the VOC, NO_x, and CO emission inventories including biogenic emissions;

The mathematical assumptions needed to integrate the differential equations formulated within OZIPM-4; and

The interpolations needed to generate isopleths from the results of a number of computer simulations.

Because these considerations are part of the basic definitions and concepts that constitute OZIPM-4 and EKMA, they are explained more fully in the following sections.

1.3 BASIC DEFINITIONS

1.3.1 Kinetic Mechanism

A kinetic mechanism is a set of chemical reactions and rate constants that is intended to describe some chemical process. Using a kinetic mechanism, one can derive coupled, first-order, ordinary, nonlinear differential equations that describe the rates of change of pollutant concentrations with time. These equations can then be integrated using a computer to simulate the changing pollutant concentrations in a smog chamber or in the atmosphere.

The original version of EKMA (OZIPP) used a two-hydrocarbon/NO_x mechanism to describe the photochemical formation of ozone (Dodge, 1977). In that mechanism, propylene and butane are used as surrogates to represent the urban mix of emissions. The propylene-to-butane ratio of 1:3 in that mechanism cannot be adjusted to account for the changing reactivity of the urban hydrocarbon mix. Because of this and other shortcomings of the original OZIPP program, many users indicated the need for a more flexible chemical mechanism. Such a mechanism was provided by Killus and Whitten (1984) with a version 3 of the carbon bond mechanism (CBM-3). Recently, an expanded version of CBM-3, called the extended carbon bond mechanism (CBM-X), was developed. This mechanism was incorporated in OZIPM3 as the default chemical mechanism. The CBM-X was consolidated to form the CBM-4 (Whitten and Gery, 1986) for use in regional oxidant models. Comparisons made using OZIPM3 with CBM-X and CBM-4 indicate close agreement (Gery, et al., 1988). Therefore, the less resource-intensive mechanism (CBM-4) has been selected for use in OZIPM-4.

Use of a mechanism such as the carbon bond mechanism (CBM-4) in OZIPM-4 instead of the Dodge propylene/butane mechanism has the following advantages:

(1) The CBM-4 is more responsive to a wider range of reactivity than is the Dodge mechanism.

(2) Reactivity is difficult to define as a function of propylene and butane if such reactivity is to be related to changes in the ambient mix of hydrocarbons.

Use of the CBM-4 in OZIPM-4 instead of the CBM-3 mechanism has the following advantages:

(1) The CBM-4 is based on more recent measurements of rate constants.

(2) The CBM-4 has been validated with more extensive smog chamber data than has the CBM-3.

(3) CBM-4 corrects errors made in computing photolytic rates in CBM-3.

1.3.2 Precursors of Ozone

Precursors of ozone are the chemical species that react to form ozone. The primary precursors are organic compounds and oxides of nitrogen (NO_x). The EPA guidelines (EPA, 1981) on the use of city-specific EKMA contain two definitions of organic compounds. The first definition, termed "VOC" or volatile organic compounds, represents the sum of the reactive organic emissions included in emission inventories. The second definition, termed "NMOC" or nonmethane organic compounds, represents ambient measurements of all organic compounds other will be termed "NMOC." NO_x, as used in this report, signifies the sum of the concentrations of nitric oxide (NO) and nitrogen dioxide (NO_2).

1.3.3 Simulation

A computer simulation involves the calculation of the concentrations of pollutants found in the kinetic mechanism as a function of time. Concentrations are calculated at various times specified by the user. The calculations involve the integration of a set of coupled, first-order, nonlinear, ordinary differential equations defined by the kinetic mechanism that describe the chemical and physical processes underlying the model. User-specified assumptions about initial precursor concentrations, emission patterns, dilution, transported pollutants, reactivity, and light intensity are incorporated in each simulation.

1.3.4 Ozone Isopleth Diagram

An ozone isopleth diagram, as generated by OZIPM-4, is illustrated in Figure 1. Each curved line in the diagram represents a constant, maximum, 1-hour average ozone concentration. Thus, the NMOC and NO_x coordinates associated with any point on a single, curved line produce the same maximum concentration of ozone. In OZIPM-4, 121 simulations are normally performed to produce such a diagram.

1.3.5 Reactivity

This is a property of the precursors that governs the rate and extent of ozone production. In regulatory applications of OZIPM-4, reactivity is determined by the sequence of reactions and reaction rate constants in CBM-4 and by the blend of NMOC species which the user of OZIPM-4 specifies as input.

1.3.6 Biogenic Emissions

Vegetation emits hydrocarbons, especially during the day. The rate of emission increases significantly with increasing temperature. These emissions also contribute to the formation of ozone.

1.3.7 Default Values

Certain parameters are needed to run OZIPM-4. Default values are levels of these parameters assumed by the computer program in the absence of instructions, by the user, to the contrary. Such instructions are entered as input data. For example, the default value for the highest NMOC used in the construction of an isopleth diagram is 2.0 ppmC. If no number is entered in the input data for this parameter, OZIPM-4 will use 2.0 by default.

1.3.8 Diagram Point

Any point on an ozone isopleth diagram generated by OZIPM-4 is associated with three parameters: initial NMOC and NO_x precursor concentrations, and a maximum 1-hour average ozone concentration corresponding to the initial NMOC and NO_x concentrations. A set of these three parameters is termed a diagram point. The ozone concentrations at some diagram points are determined from actual computer simulations (i.e., by integrating the set of differential equations). The ozone concentrations at other diagram points are interpolated from the simulated diagram points.

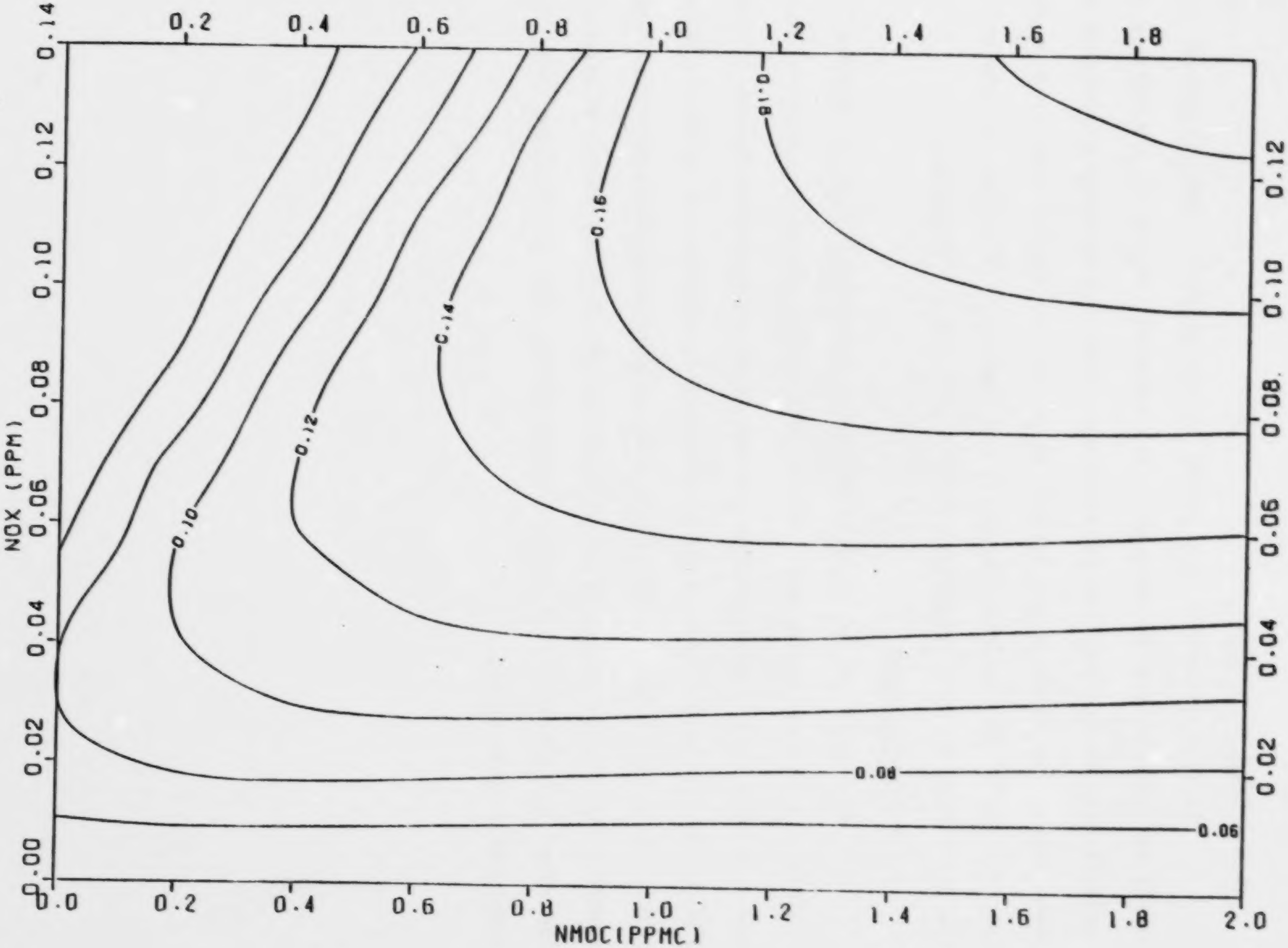

FIGURE 1. OZIPM4 EXAMPLE ISOPLETH RUN

1.3.9 Spline Interpolation

Spline interpolation is used to determine the ozone concentrations between diagram points for which ozone concentrations have been calculated by computer simulations. (Interpolation is used to reduce the number of computer simulations necessary to construct an isopleth diagram and hence to reduce the cost of running OZIPM-4.) A spline function is similar to a wire constrained to touch certain points. If the wire is pulled taut, it will bend at each point, but will be straight between points. If the tension is reduced, the wire will provide a smooth curve that touches the points. The hyperbolic spline functions used to interpolate between calculated diagram points in OZIPM-4 have an adjustable tension factor analogous to the tension on a wire. Interpolations are performed internally by OZIPM-4, and usually there is no need for the user to be directly concerned with the spline functions.

1.4 SUMMARY OF INPUT DATA

Input parameters that can be specified by the user when performing an OZIPM-4 calculation include:

Latitude;

Longitude;

Time zone;

Date;

Morning and afternoon mixing heights (also called mixing depths);

Hourly temperature variation;

The simulation start and stop times;

Initial CO concentration;

Concentrations of NMOC, NO_x, CO, ozone, and up to ten other species in the air above the mixed layer due to transport aloft (note that these cannot be varied in time);

Concentrations of NMOC, NO_x, CO, ozone, and up to ten other chemical species transported in the surface layer;

VOC, CO, and NO_x emissions at each hour;

Organic reactivity Three reactivities can be specified: background, initial, and aloft. However, each type of reactivity is fixed in time for each diagram point and at every point on the diagram; and NO_x reactivity (initial fraction of NO_x that is NO_2.)

Biogenic emission rates and speciation; and

Hourly atmospheric moisture estimates.

1.5 OUTPUT OPTIONS

The major function of OZIPM-4 is to calculate estimated NMOC reductions needed to achieve the ozone air quality standard. The output depends on the option selected by the user. Three types of output can be requested:

(1) Estimate ozone concentrations as a function of time for a single set of precursor conditions (CALC routine).

(2) Compute VOC emission reduction needed for a particular case without generating an O_3 isopleth (EKMA routine).

(3) Generate an O_3 isopleth diagram (ISOPLETH routine).

2.0 TECHNICAL DISCUSSION

The OZIPM-4 is a trajectory-type model designed to simulate ozone formation in urban atmospheres. The model consists of two distinct parts: the first part combines meteorological assumptions with a chemical kinetic mechanism to mathematically simulate physical and chemical processes taking place in the atmosphere. The second part uses the simulation results to calculate effects of a control strategy for a specific test case or to construct an ozone isopleth diagram. This chapter describes the conceptual basis for the kinetics model and the mathematical techniques used in performing a simulation.

2.1 CONCEPTUAL BASIS FOR THE OZIPM-4 MODEL

In the OZIPM-4 model, a column of air containing ozone and precursors is transported along an assumed straightline trajectory. The trajectory is defined so that the simulated column of air being modeled is positioned over the center of the city at 8 a.m. and arrives at the site observing the daily maximum O_3 concentration at the time of the observed maximum. As the column moves, it encounters fresh precursor emissions that are mixed uniformly within the column. The column is assumed to extend from the earth's surface through the mixed layer. The assumed horizontal dimensions of this column are such that the concentration gradients are small enough to make the horizontal exchange of air between the column and its surroundings insignificant. The air within the column is assumed to be uniformly mixed at all times.

At the beginning of a simulation, the column is assumed to contain some specified initial concentrations of NMOC, NO_x, and CO. As the column moves along the assumed trajectory, the height of the column can change because of variations in mixing height; it is assumed to change with time during a user-selected period (for example, 8 a.m. - 3 p.m.), and to be constant before and after that period. As the height of the column increases, its volume increases, and air above from the inversion layer is mixed in. Pollutants above the mixed layer are described as "transported above the surface layer" or "transported aloft." Any ozone or ozone precursors above the mixed layer that are mixed into the column as it expands are assumed to be rapidly mixed throughout the column.

Concentrations of NMOC species, NO, NO_2, CO, and O_3, within the column are physically decreased by dilution due to the rise in mixing height, and physically increased both by entrainment of pollutants transported aloft and by fresh emissions. All species react chemically according to the kinetic mechanism selected (i.e., CBM-4). Certain photolysis rates within that mechanism are functions of the intensity and spectral distribution of sunlight, and they vary diurnally according to time of year and location.

The following assumptions and specifications describe the OZIPM-4 trajectory model:

> The air mass of interest is an imaginary air parcel (column) of fixed horizontal area at a diurnally varying but internally uniform temperature, within which pollutants are well mixed.
>
> The region of the atmosphere containing the imaginary column is sufficiently homogeneous that horizontal diffusion does not affect pollutant concentrations within the column.
>
> The height of the column varies with time as specified by the user.
>
> The column contains specified initial concentrations of NMOC, NO_x, and CO at the simulation starting time.
>
> Pollutants transported within the surface layer from outside the area of interest may be present in the column at the start of each simulation. The pollutant concentrations due to transport in the surface layer are normally assumed to be zero, but the user may specify other values for the NMOC, NO_x, CO, and ozone concentrations transported within this layer.
>
> The changes in pollutant concentrations within the column are calculated by computer simulation for a user-specified period.

Entrainment of pollutants transported aloft is possible during the rise of the mixed layer. OZIPM-4 permits entrainment of NMOC, NO_x, CO, ozone, and a limited number of other species, but the concentrations in the layer aloft cannot be varied in time.

Pollutants emitted into the column after the starting time can be represented by specifying additions of VOC, NO_x, and CO during each hour.

Zero cloud cover is assumed.

2.2 COMPUTATIONAL PROCEDURES

This section presents a detailed description of the mathematical procedures used in OZIPM to calculate the maximum 1-hour average ozone concentration that results from a given set of initial concentrations of NMOC, NO_x, and CO, fresh emissions, transport, and meteorological assumptions. These procedures are based on the physical and chemical processes described in the last section. Before the beginning of a simulation, data-preparation steps are performed by the program. A simulation is conducted by first determining concentrations at the starting time and then numerically integrating the equations that form the basis of the chemical kinetics model included in OZIPM-4. The numerical solution yields species concentrations as a function of time continuously throughout the simulation period. The following discussion describes the data-preparation steps, calculation of initial concentrations, model formulation, and the numerical integration technique used.

2.2.1 Data-Preparation Steps

The OZIPM-4 program performs a data-preparation step before the first simulation begins. The purpose of this step is to eliminate abrupt changes in photolytic rate constants and emission rates. Elimination of these abrupt changes (i.e., discontinuities) is desirable for three reasons:

(1) The integration scheme requires less computer time (discontinuities require the use of small time steps).

(2) The results are more accurate numerically (stepping past discontinuities can lead to errors).

(3) The atmosphere does not normally have discontinuities. (The simulation of intermittent cloud cover or sudden changes in emissions is outside the scope of OZIPM).

The rate constant for NO_2 photolysis depends on the sun's zenith angle[*] and is evaluated every hour using an algorithm developed by Schere and Demerjian (1977). The algorithm uses latitude, longitude, time zone, and date as input data to calculate photolytic constants. A set of third-order polynomial spline functions is then generated so that the photolytic constant for NO_2 can be easily calculated from a smooth curve for any time of the day. For a given zenith angle, all other photolysis constants used in OZIPM-4 are estimated as described by Jeffries and Sexton (1987).

Emission rates are expressed as emission densities for each hour. The emission rates are converted to continuous functions for use in solving the differential equations through a histogram-fitting algorithm described by Jeffries, Sexton, and Salmi (1981).

2.2.2 Determination of Initial Concentrations

Before a simulation can begin, the concentrations of all pollutant species at the starting time must be determined by the program. These concentrations are derived from the initial concentrations of NMOC and NO_x that are specified by the user. The concentrations of transported pollutants are assumed to be zero unless otherwise specified by the TRANSPORT option (see Section 3). The initial CO concentration is assumed to be 1.2 ppm unless otherwise specified by the CREDIT option.

---

[*] Zenith angle is the angle between the sun's position and vertical.

Initial concentrations of biogenic species should be set to some small value (i.e., 0.0001 ppmC).

The concentrations of the nonzero species are determined by the program in the following manner:

(1) NO_2 is set to the initial NO_x concentration multiplied by the NO_2/NO_x fraction (default is 0.25).

(2) NO is set to the initial NO_x concentration multiplied by the quantity one minus the NO_2/NO_x fraction.

(3) O_3 is set to the concentration transported in the surface layer or to the background value, whichever is larger (default is zero).

(4) The concentrations of the organic species are determined from the assumed initial NMOC concentration and the assumed reactivity fraction. Mathematically,

$$[\text{organic}]_i = [\text{NMOC}]\ (R_i)/C_i \qquad (2\text{-}1)$$

where

[organic]i = i-th organic species in ppm

[NMOC] = initial NMOC concentration, ppmC

R_i = carbon fraction of initial NMOC that is species i

C_i = number of carbon atoms in species i

2.2.3 Mathematical Formulation of Kinetics Model

The kinetics model in OZIPM-4 mathematically simulates physical and chemical processes taking place in the atmosphere. This simulation is accomplished by numerically integrating a system of ordinary differential equations that describe the effects of these processes on pollutant concentrations. The result gives the concentration of pollutants as a function of time. The mathematical formulation of the system of differential equations is described next.

In OZIPM-4, four processes are assumed to affect changes in pollutant concentrations using a specific time increment:

(1) Chemical reactions;

(2) Dilution;

(3) Entrainment of pollutants transported aloft; and

(4) Emissions.

Differential equations are used to describe the time rate of change of pollutant concentrations due to each process. The total time rate of change of each pollutant concentration is then simply equal to the sum of all these effects. Thus, the system of equations consists of one differential equation for each species in the kinetic mechanism. The four processes are described next.

Chemical Reaction Effects--

The change in pollutant concentration due to chemical reaction is a function of the rates of the chemical reactions. The rate of each reaction is the product of a rate constant and a concentration term. Photolytic rate constants are calculated using procedures described by Jeffries and Sexton (1987). These procedures will be briefly summarized later. The concentration term for unimolecular or pseudo-first-order reactions (such as photolytic reactions) is simply the concentration of the reactant. Bimolecular reaction rates are calculated similarly, except that the concentration term is the product of the two reactant concentrations.

For example, the reaction rate (RT) for the reaction,

$$NO + O_3 \rightarrow NO_2 + O_2, \qquad (2\text{-}2)$$

would be expressed as

$$(RT)_2 = k_2 C_{NO} C_{O_3}$$

where

$(RT)_2$ = rate of reaction 2, ppm min^{-1}

k_2 = rate of constant for reaction 2, ppm^{-1} min^{-1}

C_{NO} = concentration of NO, ppm

C_{O_3} = concentration of O_3, ppm

If the rate constant varies as a function of temperature, then k_2 would be represented by the rate constant at 298 K, along with an activation energy (E), in deg K, such that

$$k_2 \text{ (at temperature T)} = k_{298} \times \exp\left[E/R\left(\frac{1}{298} - \frac{1}{T}\right)\right]$$

The time rate of change of a species due to chemical reaction is simply equal to the sum of all rates for those reactions in which the species is a product minus the sum of the rates for those reactions in which the species is a reactant. Thus

$$\left[\frac{dC_i}{dt}\right]_R = \Sigma(RT)_{PROD} - \Sigma\,(RT)_{REAC} \qquad (2\text{-}3)$$

$\left[\frac{dC_i}{dt}\right]_R$ = chemical reaction contribution to the time rate of change of species i

$\Sigma(RT)_{PROD}$ = the sum of all reaction rates in which species i appears as a product

$\Sigma(RT)_{REAC}$ = the sum of all reaction rates in which species i appears as a reactant

Dilution Effects-

The mathematical representation for simple dilution due to changes in the mixing depth is a first-order decay process. The rate of change due to this effect can be represented as follows:

$$\left[\frac{dC_i}{dt}\right]_D = D_t C_i \qquad (2\text{-}4)$$

where

$\left[\frac{dC_i}{dt}\right]_D$ = dilution effect contribution to the time rate of change of pollutant species i, ppm $\min^{-1}$

D_t = dilution factor, $\min^{-1}$ (function of time),

C_i = concentration of species i, ppm.

The dilution factor is calculated by assuming that the mixing height varies from a minimum (or morning) mixing height to a maximum (afternoon) mixing height in accordance with a "characteristic curve" derived empirically from data taken during the St. Louis RAPS study (Schere and Demerjian, 1977). The "characteristic curve" represents the fractional growth in mixing height as a function of the fraction of daylight. The fraction of daylight is calculated as follows:

$$\text{Fraction of daylight} = \frac{\text{Time (current)} - \text{(time of sunrise)}}{\text{(time of sunset)} - \text{(time of sunrise)}}$$

The mixing height at any given time is:

$$\text{Mixing height} = H_0 + F_G \times DH$$

where

H_0 = mixing height at time of sunrise (calculated from the minimum mixing height)

DH = maximum mixing height - H_0

F_G = fraction of growth in mixing height.

The "characteristic curve" is depicted graphically in Figure 2. Note that before and after the inversion rise period, the dilution factor is zero since there are no dilution effects for those periods.

Two modifications have been made to the characteristic curve concept to facilitate its use. First, a smooth curve through the points shown in Figure 2 is used to avoid discontinuities. Secondly, the mixing height at the start of the simulation (usually 0800 hours) is used instead of H_0 as noted above since most simulations start after sunrise.

Entrainment Effects--

Pollutants above the mixed layer are subject to entrainment into the column of air simulated by the model. In OZIPM-4, these may be NMOC, NO_x, O_3, and up to 10 other chemical species. The mathematical treatment of entrainment assumes that the concentrations aloft do not change with time and that they extend uniformly to at least the height of the afternoon mixed layer. The pollutants entrained are assumed to mix rapidly within the enlarged surface layer. The mathematical expressions for the rates of change of the pollutants are shown by the following equations:

$$\left[\frac{dC_i}{dt}\right]_{AL} = D_t(C_i)_{AL} \qquad (2\text{-}5)$$

$$\left[\frac{dC_{HC_j}}{dt}\right]_{AL} = D_t(C_{NMOC})_{AL}\ R_{HC_j}/C_j \qquad (2\text{-}6)$$

where

$\left[\frac{dC_i}{dt}\right]_{AL}$ $\left[\frac{dC_{HC_j}}{dt}\right]_{AL}$ = the contribution of entrainment to the time rates of change of species i or hydrocarbon species j, respectively, ppm min^{-1}

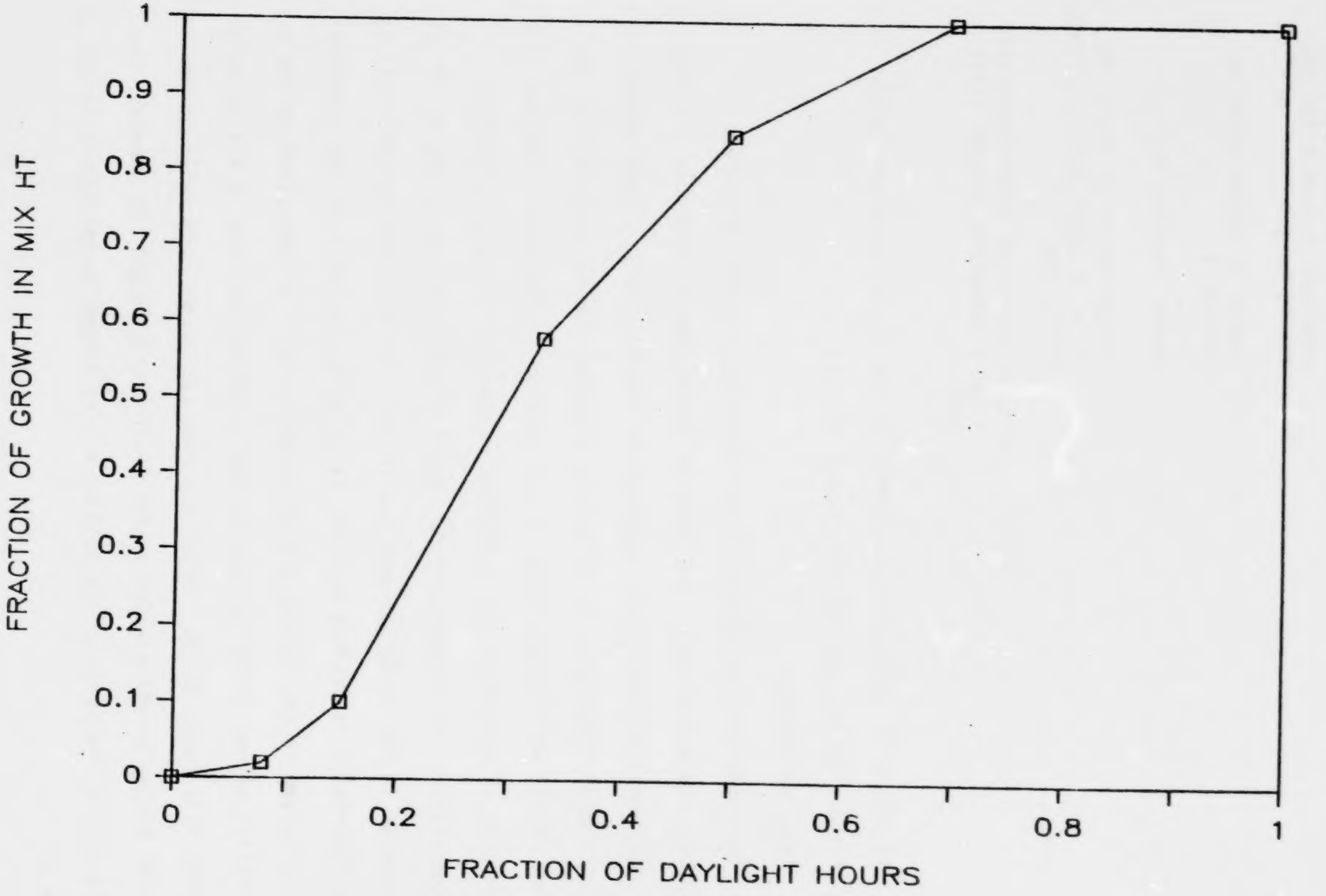

FIGURE 2. CHARACTERISTIC CURVE

D_t = dilution factor (i.e., the rate constant at time t for the mixing height rise), min^{-1}

C_j = number of carbon atoms in species j

$R_{HC\,j}$ = carbon fraction of $C_{HC\,j}$

$(C_i)_{AL}$ = concentration of ozone, NO_2, and up to 10 other species trapped aloft, ppm

$(C_{NMOC})AL$ = concentration of total nonmethane organic compounds trapped aloft, ppmC.

It should be noted that the effect of the change in mixing height is the sum of the dilution and the entrainment effects.

Emission Effects-

Emissions are the fourth factor affecting the rate of change of pollutant concentrations. The rates of change due to emissions are equal to the additional concentrations produced by the emissions. These concentrations are estimated internally in OZIPM-4 by dividing the emission rate by the volume in the well mixed column of air assumed in the model. Because equal quantities of emissions into different volumes will produce different concentrations, it is necessary to adjust the relative emissions to reflect the change in the column volumes due to the rise in mixing height. This is done internally in OZIPM-4 by first calculating the ratio of the starting mixing height to the current mixing height. (This is equivalent to the ratio of initial volume to the current volume.) Before the rise in mixing height begins, this ratio is one. After the rise has ceased, the ratio is the initial mixing height divided by the final mixing height. In general, the ratio (f_t) is the ratio of the initial mixing height to the mixing height at time t.

The rates of change due to the emissions are calculated from the values of the emission rates, the f_t ratio just described, and the reactivity inputs. The equations for the rates of change due to emissions for each of the affected species are shown below:

$$\left[\frac{dC_i}{dt}\right]_E = f_t\ (E_i)_t,$$

where

$\left[\frac{dC_i}{dt}\right]_E$ = emission contribution to the rates of change of species i, ppm min^{-1}

$(E_i)_t$ = value of emission rate, ppm per minute

For these formulations, a conversion from ppmC to ppm is performed for hydrocarbon species, and the reactivity of the hydrocarbons is taken into account.

Carbon monoxide emissions can be treated explicitly using the option. (CREDIT), discussed in Section 3.

2.2.4 Description of Numerical Integration

The kinetics model in OZIPM-4 employs a Gear-type integration scheme to numerically solve the set of differential equations described in the previous section. This procedure has been described elsewhere (Gear, 1971; Spellman and Hindmarsh, 1975; Sherman, 1975). The integration scheme initially uses a time step of 1×10^{-10} minutes (i.e., pollutant concentrations are to be calculated 1×10^{-10} minutes after the start time). Subsequent time step sizes are then computed by the Gear-type integration scheme according to the estimated error at each step. The pollutant concentrations are calculated at each time step throughout the simulation period. (Once the final hour is reached, there is no restriction on precisely matching the final time step, since the concentrations can be interpolated back to exactly the last hour.) A typical simulation period takes from 150 to 200 time steps; about one half of these time steps are used in simulating the first minute.

The total rate of change of any species is the sum of the rates of change due to dilution, entrainment, emissions, and chemical reaction just described. At each time step, the concentrations of all species are calculated along with the current rates of change for each species to predict the species concentration at the end of the time step using a Taylor-series type polynomial. The order of the polynomial is varied internally for optimum efficiency and is based on the values at the beginning of the time step. A corrective scheme then "corrects" the new concentration values, updates the Taylor polynomials, and estimates the average error. The corrector is a set of linear equations based on a Jacobian matrix whose elements are the set of partial derivatives of rates of change of concentrations of each species with respect to each of the other species. OZIPM-4 utilizes a linear system solving package for sparse matrices (i.e., those matrices in which most elements are equal to zero).

The integration method used in OZIPM-4 has been modified somewhat from the version published by Spellman and Hindmarsh (1975). For example, the error estimation is performed relative to the current concentration of a species rather than relative to its maximum concentration. The method utilizes the error estimate to determine the optimum step size and order, so that the allowable error specified by the user is met with the minimum number of integration steps.

The final task performed during the integration of the differential equations is determination of the maximum 1-hour-average ozone concentration. Ozone concentrations are calculated for every minute of the simulation. This calculation is performed by interpolation between the actual time steps used in the integration. Running 1-hour average concentrations are calculated using Simpson's rule and are updated every minute. The largest 1-hour average concentration is then selected as the maximum.

2.3 SELECTION OF SIMULATIONS FOR GENERATION OF ISOPLETH DIAGRAMS

When generating an ozone isopleth diagram, the initial NMOC and NO_x concentrations for each simulation are selected internally by OZIPM-4. The program controls the selection of NMOC and NO_x concentrations so that maximum accuracy is obtained for the isopleth diagram for a given number of simulations.

The OZIPM-4 performs a series of 121 simulations on an 11 x 11 rectan-gular grid with points evenly spaced within the specified range of NMOC and NO_x concentrations. From these 121 simulations, the pollutant isolines are estimated based on contouring procedures described by Sutcliffe (1978).

3.0 DESCRIPTION OF OZIPM-4 OPTIONS

This section describes in detail the different options and inputs available for use with the OZIPM-4 computer code. Only options which are anticipated for use with regulatory analyses are listed below.

City-Specific Options

PLACE - location of the site

DILUTION - input minimum and maximum inversion heights

TEMPERATURE - input hourly temperature values

TRANSPORT - input surface layer and aloft conditions of NMOC, NO_x, and O_3

MASSEMISS - input hourly mass emission densities of VOC and NO_x

REACTIVITY - input reactivity of the initial NMOC mix and VOC emissions and the initial NO_2/NO_x ratio

CREDIT - input hourly emission densities of CO and allow change in CO in the future year.

BIOGENICS - input hourly mass emission densities of biogenic emissions

WATER - input hourly relative humidities (needed to estimate atmospheric moisture content)

Additional Simulation Options

TITLE - input simulation title

TIME - input starting and ending times for computer simulations

SPECIES - input the species of interest for isopleths

ACCURACY - change the accuracy of the simulation (error tolerance) and the tolerance for spline interpolation

ALREADY - time saving option utilizing simulations from a previous run

PLOT - do off-line plotting (CALCOMP)

Program Output Options

EKMA - perform calculations to obtain required VOC reduction, given assumptions about changes in NO_x and CO

CALCULATE - do a single point on the isopleth, calculating ozone as a function of time

ISOPLETH - do the whole isopleth diagram

The first four letters of each option have been underlined to denote the required input code. Typical OZIPM-4 simulations for regulatory analyses are expected to contain the following options: PLACE, DILUTION, TEMPERATURE, TRANSPORT, MASSEMISS, REACTIVITY, CREDIT, TITLE, BIOGENICS and WATER. Depending upon the type of simulation, the following options may also be included: EKMA, CALCULATE, ISOPLETH, and PLOT. Example runs are contained in the appendices.

3.1 SITE-SPECIFIC OPTIONS

Several options can be used to describe the initial and meteorological conditions for the computer simulations. These options are PLACE, DILUTION, WATER, TEMPERATURE, TRANSPORT, and TIME. Three different options MASSEMISS, CREDIT, and BIOGENICS can be used to describe the emissions entering the air parcel during the simulation. The option REACTIVITY is used to specify site-specific information on the reactivity of the initial NMOC and NO_x ambient mix and the VOC and NO_x emissions.

3.1.1 Place and Date

In all OZIPM-4 runs, the rate constants of the photolysis reactions in the kinetic mechanism are varied in accordance with the diurnal change in sunlight intensity (or solar zenith angles) during the specified simulation period. This diurnal variation is calculated using a computer code written by Schere and Demerjian (1977) that is incorporated in OZIPM-4. The user can adjust the photolysis rate constants to the area of interest by changing the date or location, or both, from the default values of 21 June 1986 at Los Angeles, California. The option is activated by the code word PLACE. The first three numeric fields of the PLACE line (Columns 11 through 40) contain the latitude (decimal degrees north), longitude (decimal degrees west), and time zone (hours from Greenwich Mean Time). The next three fields are used to specify the year, month, and day in Columns 41-50, 51-60, and 61-70, respectively. An additional line may be required after the PLACE line. On this line, the name of the city of interest is entered between Columns 1 and 24. This line is necessary only if a nonzero value for the latitude or the longitude is entered on the PLACE line. Therefore, even if the default values of 34.058 and 118.250 are entered, a second line is required with the name of the place. Users interested in the default location need not specify the latitude and longitude.

The correct set of numerical time zones for the continental United States is as follows:

Numerical Time Zone	Common Name
4.0	Eastern Daylight Time
5.0	Central Daylight Time
6.0	Mountain Daylight Time
7.0	Pacific Daylight Time

To produce standard time simulations, even though the output will show daylight time units, a false time zone can be created by increasing the numerical time zone by one unit (hour). Thus, Pacific Standard Time photolysis constants would be generated if a 8.0 were entered instead of the correct 7.0 time zone. The output should then show that solar noon occurs near 1200 hours when the printing of solar noon is activated.

3.1.2 Dilution Rate

Dilution in OZIPM-4 occurs as a result of the rise in the early morning inversion. Under default conditions, the mixing height is assumed to rise from 510 meters to 630 meters over a 7-hour period starting at 0800 LDT using the characteristic curve.

City-specific values for determining the characteristic-curve dilution rate are entered using the word DILUTION. The values of the morning mixing height, afternoon mixing height, starting time for the rise in mixing height, and stopping time for the mixing height rise are entered in the first four numeric fields of the DILUTION line (i.e., Columns 11-20, 21-30, 31-40, and 41-50, respectively). The starting and stopping time should be in 24-hour time format, LDT. For both default and specific conditions, dilution is assumed not to occur outside the starting and stopping times.

3.1.3 Temperature

Another option found in OZIPM-4 is the variation in temperature during a simulation period. The chemical kinetic mechanism can be dependent on the variation of temperature in the manner described by Whitten, Killus, and Hogo (1980). As the temperature rises, the kinetic mechanism generally reacts more rapidly, leading to earlier formation of ozone during the simulation period and possibly higher amounts of ozone. The user declares this option (TEMP) and gives the number of hours of temperature data to input. The temperatures are then entered for the initial hour and the end of each hour. All temperature values must be in units of degrees Kelvin. If the TEMPERATURE option is not used, the default value is 303°K, which is assumed to be constant throughout the simulation.

3.1.4 Atmospheric Moisture

In the past, OZIPM-4 has used a constant default water vapor concentration of 20,000 ppm. However, recent work has shown that predicted ozone levels can vary by as much as 20 to 30 percent with factors of two variation in water vapor concentration. The WATER option is used to input the daily atmospheric pressure and hourly values of the relative humidity. OZIPM-4 will calculate hourly values of water vapor concentration used in the model simulations.

3.1.5 Initial Conditions of Transported Species

The TRANSPORT option is used to input initial concentrations of O_3, NMOC, and NO_2 transported in the surface layer and entrained from aloft. The concentrations of transported O_3 and NO_2 are entered on the first line of the TRANSPORT option. Transported NMOC concentrations are also entered on the first line if the default compositions for surface and aloft NMOC transport are used. However, if the user wants to change the composition of transported NMOC from the default values, the format for the NMOC inputs is different. Instead of entering the concentration for NMOC transported in the surface layer, a "-9" is entered in that field on the TRANSPORT line. Similarly, a "-9" is entered if there are organics entrained from aloft. These numbers correspond to the number of transported organic species in the CBM-4. Immediately following the TRANSPORT line the concentration of NMOC transported in the surface layer and the fraction of the total organic for each organic species are input. Similarly, the concentration of NMOC aloft and the fraction of the total NMOC for each organic species are input on the third line of the transport option (or immediately following the TRANSPORT line if there is no surface transport of NMOC). Note that the fractions for the organic species transported in the surface layer and aloft can be different in the two cases. When using CBM-4, the fractions must be entered in the following order: ETH, OLE, ALD2, FORM, TOL, XYL, PAR, ISOP, and NR.

The concentrations of species transported in the surface layer and aloft remain constant for any simulation on a given isopleth diagram. The EKMA option is the only option which allows the user to modify transported surface and aloft conditions for future year calculations without having to perform a separate, new model run.

3.1.6 Simulation Starting and Ending Times

Optional starting and ending times can be entered with the TIME option. The starting and ending times (Local Daylight Time, based on the 24-hour clock) are placed in the second (Columns 11-20) and third (Columns 21-30) ten-column fields, respectively. Times may be entered to the nearest minute, but the time difference (stop minus start) must not exceed 24 hours. Both the starting and ending times are set back to default values when a zero value is entered for the ending time.

Starting and ending times can also extend beyond midnight into the next day; the user need only specify the times. Thus, the maximum of 24 hours for a simulation is not confined to a 24-hour period from midnight (0000 hr) to 2400 hours.

3.1.7 Emissions

The MASSEMISS option allows the user to input VOC and NO_x emissions in units of kg/km^2. The hourly emission densities are converted to fractions of initial concentrations within the program based on the initial NMOC and NO_x concentrations, and the initial mixing height (in meters). This procedure is described in EPA (1989). The first MASSEMISS line contains the number of hours emissions are to be added, the initial NMOC and NO_x concentrations, and the beginning mixing height. The next line contains up to 7 hours of VOC emissions in kg/km². The following lines either continue VOC emissions or NO_x emissions.

3.1.8 Consideration of Carbon Monoxide

The CREDIT option allows for post-8 a.m. CO emissions in EKMA calculations. The first line of the CREDIT option contains the number of hours emissions are to be added, expressed as a negative number. This number must match the number of hours on the MASS option. The initial mixing height is also entered on this line. The second line contains the present-day 6-9 a.m. CO concentration, the present-day CO concentration in the surface layer, the present-day CO aloft, the percent change in CO emissions for the future year, future CO in the surface layer, and future CO aloft. The third line contains hourly emissions of CO in mass units. If the user inputs a present-day 6-9 a.m. CO concentration, that value will be reduced in the future-year calculations by the percent change in CO emissions that is entered for the future year.

3.1.9 Biogenic Emissions

The BIOGENICS option is used to input post-0800 emissions of up to five biogenic species. The CBM-4 mechanism treats one biogenic species (isoprene) explicitly. Other biogenic species are expressed as CBM-4 species according to the methodology outlined in EPA (1989). The first line in the BIOGENICS option contains the four letter code "BIOG" to invoke the BIOGENICS option followed by the number of hours of emissions of the biogenic species. Note, a negative number of hours is entered to be consistent with the MASS option. The third item on the first line is the number of biogenic species with post-0800 emissions. Up to five biogenic species can be input. The initial mixing height (in meters) is entered next. The mixing height is used to convert hourly emission densities to concentration units required by the OZIPM-4 program.

The next set of lines (lines 2 to 5) are repeated for each biogenic species up to the number specified in columns 21-30 of the first line. The second line of the BIOGENICS option contains the name of the biogenic species. The only biogenic species which requires an exact spelling is isoprene (ISOP) since it is a species found in the photochemical mechanism. Note that ISOP must be in capital letters. The next item (located in columns 11-20) on the second line contains a flag to tell OZIPM-4 that the species is treated explicitly in the photochemical mechanism. A nonzero positive value would tell OZIPM-4 that the species is to be treated as a mixture of CBM-4 species. Currently, for isoprene, the flag would be set to zero. The next items on line 2 are the present-day biogenic concentrations transported in the surface layer and entrained from aloft (in units of ppm). The percent change in biogenic emissions for the future year is entered next, followed by the future-year concentrations transported in the surface layer and entrained from aloft.

The third line of the BIOGENICS option contains the species molecular weight in units of gm/mole. If the flag located in columns 11-20 of line 2 is nonzero, the next lines contain the species bond fractions apportioned to the CBM-4 species. The bond fractions must be input in the following order: ETH, OLE, ALD2, FORM, TOL, XYL, PAR, and NR.

The next set of lines in the BIOGENICS option contains the hourly emission densities in units of kg/km^2. Note, the BIOGENICS option can be used to input only initial and aloft biogenic concentrations by entering small emission densities (e.g., 0.0001) for each of the hours of emissions.

3.1.10 Reactivity of Initial Mix and VOC Emissions

Organic reactivity and the initial NO_2/NO_x ratio for both the 0600--0900 ambient mix and the VOC and NO_x emissions are input with the REACTIVITY option. The following entries must be made on the REACTIVITY line:

The number of organic species; and

The NO_2/NO_x ratio

If the number of organic species is nonzero, the next line(s) describes the fractions of the total organic (per carbon basis) that each organic species represents. The order must be the same as that for the name and carbon numbers entered earlier. The sum of the organic fractions should normally be equal to one. Note that the carbon fractions and NO_2/NO_x ratio for both the initial mix and the subsequent emissions must be identical. The default values for the organic fractions are set to the values recommended in Section 4.

3.2 OUTPUT OPTIONS

Output options are of three types:

(1) Perform a single simulation;

(2) Estimate VOC control requirements automatically without generating an isopleth diagram; and

(3) Estimate VOC control requirements by generating an isopleth diagram.

A single simulation is performed using the CALCULATE option. The second option (EKMA) estimates the VOC control requirement based on inputs of an hourly ozone concentration (generally the daily maximum value observed on the day being simulated) and $NMOC/NO_x$ ratio into OZIPM-4. The third option (ISOPLETH) requires the generation of at least one isopleth diagram in which all calculations are performed on the diagram.

All three options are discussed in detail in the following paragraphs.

3.2.1 Performing a Single Simulation (CALC)

Individual simulations can be performed at specified initial NMOC and NO_x concentrations using the CALCULATE line. The first two numeric fields on the CALCULATE line (Columns 11-20 and 21-30) specify the desired 0600-0900 ambient NMOC and NO_x concentrations. The initial conditions and hourly ozone concentrations will be printed to show the change of ozone with time during the simulation. Any number entered in the third numeric field (Columns 31-40) will activate an information option that will print:

The rate constants used in the kinetic mechanism,

The concentrations of all species in the kinetic mechanism,

The net rate of change of all species,

The reaction rates for each reaction, and

The photolysis constants for all photolysis reactions.

If the information is activated, the user can then specify the simulation time (in minutes) for which concentrations of all species, current reaction rates, etc., will be printed. The number of minutes after the simulation starting time as which the initial printing is made (default value = 60 minutes after start) is entered in Columns 41-50. The integral time step for which subsequent printings are made (default value = 60 minutes) is entered in Columns 51-60. Under default values, hourly concentrations of species, net rates of changes, etc., are printed. After the simulation has ended, a concentration versus time profile is printed for ozone.

3.2.2 Calculating VOC Control Requirements for a Specific Case (EKMA)

A feature available in the OZIPM-4 program is the ability to perform a VOC emission reduction calculation without generating an ozone isopleth diagram.

When the EKMA option is used, the user must supply information on the ozone concentration to be reduced to the level of the U. S. NAAQS (0.12 ppm), the NMOC/NO_x ratio to be used in the calculation, and the percent change in NO_x emissions. In addition, changes in CO levels should be considered. Changes in CO are considered with the CREDIT option, which should be run in conjunction with the EKMA option. The calculations in EKMA are performed in accordance with the procedures used to calculate control estimates from an ozone isopleth diagram (EPA, 1981). Through an iterative search procedure, the design point is first located by finding the initial NMOC and NO_x concentrations (with the specified ratio) that produce the desired ozone concentration (within 0.0005 ppm). A post-control point is then found by first adjusting the base-case NO_x point to reflect the change in NO_x emissions input by the user, and then finding the initial NMOC concentration that, along with the adjusted NO_x concentration, will produce an ozone value of 0.12 ppm (again, within 0.0005 ppm). The VOC reduction estimate is then calculated as the percent change in NMOC concentration from the base case point to the post-control point.

Following Gipson (1984), the EKMA option is activated by an input record with the code word EKMA located in Columns 1-4. The design ozone value is then placed in the first numeric field of the EKMA input record. The second numeric field of this record contains the NMOC/NO_x ratio. The percent change in NO_x emissions that is expected between the base case and the post-control time periods is coded in the third numeric field. This value should be entered as the percent change. Thus, a positive entry corresponds to an increase, and a negative entry, to a decrease. (For example, a 5 percent increase would be coded as 5.0, and a 5 percent decrease, as -5.0.) The fourth numeric field is used to signify a change in transport conditions. If the same transport conditions are assumed for the base case and post-control case, this entry may be left blank. Otherwise, a numeric entry (e.g., 1.0) denotes that transport conditions to be used for the post-control case are different from those used for the base case, and these new values are coded in the next input record.

The first two fields of this next input record contain the surface and aloft ozone concentrations (in ppm), respectively. If a negative value is input, then future-year ozone transport is estimated using the curves described in EPA (1989) and shown in Figure 3. As noted in EPA (1989), cities in the ROMNET domain should follow alternative procedures which are currently being developed for preparation of present and future levels of ozone and precursors aloft. The third field contains the concentration of NMOC transported in the surface layer for the post-control situation. It is recommended that this value be set to zero. The fourth field represents the concentration of NMOC transported aloft for post-control conditions. It is recommended that this value be set to 24 ppmC if the default NMOC aloft conditions are used. The next two fields (five and six) contain the future NO_x surface and aloft transport levels (in ppm). The user should note that the structure of this input record is similar to that of base-case transport level will be used for the post-control case. Also, no provisions are included for making any changes to the composition of NMOC used in the simulations (i.e., the same NMOC transport composition will be used for both base case and post-control point).

The last line of the EKMA option contains the median 0600-0900 NMOC and NO_x values, which are used internally by OZIPM-4. This line is also used to input the base-year NMOC and NO_x concentrations (in units of ppmC and ppm) in Columns 31-40 and 41-50 if the user already has this information from single

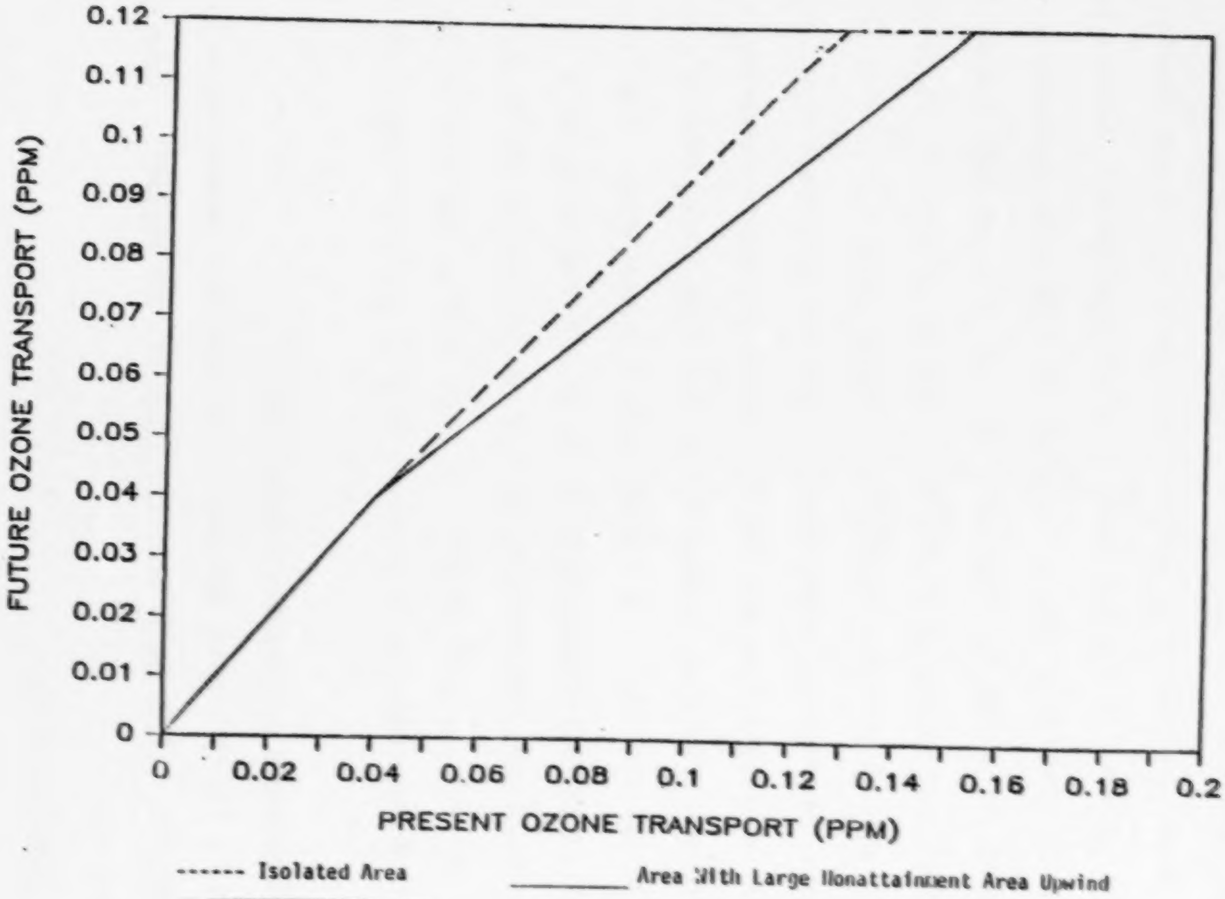

FIGURE 3

FUTURE OZONE TRANSPORT AS A FUNCTION OF PRESENT TRANSPORT

CALC runs or from previous simulations. If a negative NMOC/NO_x ratio is input, OZIPM-4 will read the base-year location and skip to the future-year control estimates. This capability saves computer time and costs.

As just described, the EKMA option causes the program to compute the VOC reduction (in percent) needed to lower the base ozone to 0.12 ppm. Another option available to the user is the ability to generate supplemental information. An entry of 1.0 in the fifth numeric field of the EKMA line generates a tabular report showing the change in ozone as a function of percentage change in VOC. Predicted ozone corresponding to VOC reductions of 10 percent, 20 percent, 30 percent, ... and 100 percent, respectively, are printed. If a value of 2.0 is coded instead, the predicted ozone concentrations will also be written to a user-defined file, which might be used for subsequent analysis or graphical display One output record is written to the file for each EKMA option that is activated. The output format consists of 11 fields, each 5 columns wide. The first field (Columns 1-5) contains the base-case ozone value. The remaining 10 fields contain the ozone predictions corresponding to the VOC reductions of 10 percent, 20 percent, 30 percent, ... 100 percent, in that order. The user can perform a single specified VOC reduction if a nonzero value is declared in the sixth numeric field.

3.2.3 Generating an Isopleth Diagram (ISOP)

Up to six additional options can be used when generating an isopleth diagram: ISOPLETH, TITLE, PLOT, SPECIES, ACCURACY, and ALREADY. These options are described next.

3.2.4 ISOPLETH Option

In all OZIPM-4 isopleth diagrams, the origin represents 0.0 initial 0600-0900 a.m. NMOC concentrations (ppmC) and 0.0 NO_x concentrations. The maximum NMOC and NO_x values represented on the abscissa and the ordinate can be changed from their respective default values of 2.0 ppmC NMOC and 0.14 ppm NO_x by putting the desired maxima into the first two numeric fields of the ISOPLETH line. The desired maximum NMOC concentration should be placed in the field of Columns 11 through 20. The desired maximum NO_x concentration should be placed in the field of Columns 21 through 30.

Any number can be used for the desired maximum NMOC and NO_x concentrations. However, because the scales on the abscissa and the ordinate are divided into ten and seven divisions, respectively, only certain values of the maximum will produce even markers. Thus, to produce an easy-to-use diagram, the NO_x maxima should be evenly divisible by seven (e.g., 0.14, 0.21, 0.28, 0.35, etc.). Similar consideration should be given to selecting an NMOC maximum.

The desired number of isopleths in the diagram should be inserted (followed by a decimal point) in the field of Columns 31 through 40 of the ISOPLETH line. Up to 20 isopleths can be drawn (the default value is 11). OZIPM-4 then reads the proper number of fields from the succeeding line or lines to provide the ozone concentrations (in units of ppm) for which isopleths are to be drawn. For example, inserting 10.0 in Columns 31-34 of ISOPLETH causes OZIPM-4 to read the seven 10-space numeric fields on the next line and three on the succeeding line. (OZIPM-4 does not read past Column 70 on any line except the program title line.)

OZIPM-4 can provide isopleth diagrams for up to five species when the SPECIES option is specified. The user must enter the number of species to be plotted in columns 61 to 70. The program will read the appropriate set of isolines to be plotted based on the value in columns 61 to 70 (one set per species). The number of isolines for each set is determined from the value entered in columns

31 to 40. The user enters the values for each set of isolines after the ISOPLETH line.

3.2.5 TITLE Option

The title can be changed by inserting a line with the word TITLE followed by a line with the desired title. Everything in Columns 1 through 72 of this title line will be printed on the output and isopleth diagrams in place of the default title, "Standard Ozone Isopleth Conditions." As with all options, these lines must precede the ISOPLETH, CALCULATE, or EKMA lines.

3.2.6 PLOT Option

Any plotting package that can be called using the standard CALCOMP subroutines can be used. Calls to these routines are activated by a line with the code word PLOT. This line must precede the ISOPLETH line. The actual CALCOMP routines called are PLOTS, PLOT, NUMBER, SYMBOL, and NEWPEN (if necessary). The use of the CALCOMP routines is discussed in Section 5.

The user also has the option to specify the actual size of the plot by defining the lengths (in inches) of the sides of the diagram. Columns 31-40 are used for the abscissa of the diagram. Columns 41-50 are used for the ordinate of the diagram. The size of title characters and axes numbers and the size of the isopleth labels can also be set by the user in Columns 51-60 and 61-70, respectively. The default values are given in Section 4. If the user wishes to reset any of these values, it is recommended that all values change proportionally.

Another option on the CALCOMP plots is the overlay of gridded lines on the isopleth diagram. This is done by declaring any nonzero positive values in Columns 21-30. If this option is exercised, a grid of different colors will be overlaid onto the diagram. If the user does not have access to the choice of different pen colors, use of this option is not recommended. If there is access to a matrix plotter (such as the VERSATEC plotter) and the choice of lines consists of thickness and pattern (i.e., dot-dash on solid patterns), the user can then enter a negative nonzero value in Columns 21-30. The absolute value of the number entered represents the user's choice of pattern and thickness. This number varies with different computer systems.

3.2.7 SPECIES Option

The OZIPM-4 package also has the capability of plotting an isopleth for any species in the kinetic mechanism. For instance, a user may be interested in plotting an NO_2 or PAN (peroxyacetylnitrate) isopleth. To activate this option, the user inputs a line with the word SPECIES in the first 10-column field and the number of species to be plotted. On the next line, the species names (or alphanumeric symbols), as used in the kinetic mechanism, are placed in the first four columns of each 10-column field (i.e., 1-4, 11-14, 21-24). The program will calculate maximum 1-hour values for the species of interest. Isopleth diagrams will be generated for all species of interest when the ISOPLETH option is used, as noted earlier. If the SPECIES line is not used, the program will be set to the default species O_3 (ozone). The SPECIES option can also be used with the CALCULATE option to generate concentration-time plots for the species of interest.

3.2.8 ACCURACY Option

The ACCURACY option controls the number of simulation points used in generating an isopleth diagram. The OZIPM-4 performs 121 simulations. Use of the ACCURACY option is not recommended for routine applications of OZIPM-4. The spline tension factors used for the spline interpolation routines are specified in Columns 41-50 and 51-60. Since the ISOPLETH option requires greater amounts of execution time, the user is advised to perform several single calculations near the maximum NMOC and NO_x concentrations to assure that the design ozone isoline occurs near the upper right portion of the diagram. Poor choices for the maximum NMOC and NO_x concentration can lead to isolines occurring off the diagram or may be compressed into a small part of the diagram.

3.2.9 ALREADY Option

Results from previous simulations can be utilized with the ALREADY option. To incorporate results from a previous run, the following conditions must be identical in both runs: the NMOC and NO_x scales, and the city-specific options. Such a situation could occur when:

- An initial run is terminated because of a time restriction;
- The user wishes to repeat the run with the PLOT option to obtain a CALCOMP-generated plot; or
- The user wishes to alter the tension factors used in the interpolation schemes;
- The user wishes to plot an isopleth for a species other than the first species specified by the SPECIES option.

To input the results of previous runs, the number of completed simulations is entered in the first numeric field (Columns 11-20) of the ALREADY option. The results of those simulations must be entered on the following lines in the same order in which they are calculated. Each line contains the results of one simulation. Field 1 (Columns 1-10) contains the initial NMOC concentration, Field 2 (Columns 11-20) contains the initial NO_x concentration, and Field 3 (Columns 21-30) contains the resulting maximum 1-hour average O_3 (or other species) concentration. If a negative number of completed simulations is entered, then OZIPM will read the completed simulation results from an external file automatically generated by the OZIPM from the previous run.

4.0 USING THE CBM-4 IN OZIPM-4

The carbon bond concept (Whitten, Hogo, and Killus, 1980) was developed mainly to simplify chemical kinetics mechanism use in atmospheric applica- tions. Therefore, the simple procedures developed for earlier versions of the carbon bond mechanism used in EKMA and published in several documents can, for the most part, be applied to the use of the CBM-4. The most recent documenta- tion for using carbon bond chemistry in EKMA can be found in Killus and Whitten (1984), Gipson (1984), and Hogo and Whitten (1985). The detailed development of the CBM-4 is documented in Gery, et al (1988).

The carbon bond mechanism (CBM-4) is actually a hybrid of explicit chemistry, surrogate approximations, and lumped/generalized chemistry designed to simulate the broad features of urban smog chemistry. Explicit chemistry is used to treat the inorganic and carbonyl species plus the chemistries of ethene, toluene, and xylene. Surrogate approximations are utilized to treat mono-substituted aromatics such as propylbenzene and di-substituted aromatics such as diethylbenzene. The carbon bond lumping method is used primarily for paraffins and olefins.

Each part of the CBM-4 chemistry, such as the inorganic subset or the ethene chemistry, conforms to current literature review studies and has been extensively tested against smog chamber data of organics/NO_x systems (Gery, et al, 1988). In addition, the entire CBM-4 was used to simulate a new series of auto exhaust and synthetic auto exhaust experiments involving a variety of conditions. Most of the smog chamber experiments used for CBM-4 testing were performed in the outdoor dual-chamber facility of the University of North Carolina, which is a well-characterized chamber with extensive analytical capabilities. The CBM-4 also successfully simulated multiple day experiments using a synthetic urban mixture of hydrocarbons performed in the outdoor dual smog chamber at the University of California at Riverside (Gery, et al, 1988).

In this section, a description of the CBM-4 and information for its use in OZIPM-4 is presented.

4.1 DEFAULT CBM-4 MECHANISM

The default chemical mechanism implemented in OZIPM-4 is the CBM-4 mechanism presented in Appendix A. The CBM-4 mechanism consists of 34 chemical species and 82 chemical reactions. The CBM-4 contains 9 primary organic species (see Table 1).

TABLE 1. CARBON NUMBERS OF CARBON BOND GROUPS FOR PRIMARY SPECIES

Carbon Bond Group	Carbon Number (carbon atoms per molecule)
PAR	1
ETH	2
OLE	2
TOL	7
XYL	8
FORM	1
ALD2	2 (acetaldehyde)
ISOP	5
NR	1

The species NR represents that portion of different molecular species treated as unreactive. Several species whose concentrations do not vary (such as O_2 and N_2) are lumped in with the rate constant. The default concentration of H_2O used in the CBM-4 corresponds to 50 percent relative humidity (20,000 ppm) at approximately 303°K.

The CBM-4 mechanism shown in Appendix A is that discussed by Whitten and Gery (1986) except that one reaction has been added. The following reaction,

$$NR \rightarrow NR \qquad k = 1\ \mathrm{min}^{-1}\ ,$$

is added to account for the nonreactive species.

4.2 DEFAULT PHOTOLYSIS RATE CONSTANTS

The CBM-4 chemical mechanism contains 11 photolysis reactions that vary with solar zenith angle (see Table 2). The photolytic rate constants for NO_2 are stored in OZIPM-4 as a function of zenith angle. These rates, which were derived by Jeffries and Sexton (1987) and Gery, et al. (1988), are the recommended j-values and are given in Table 3. The default values represent the reaction rate constants at approximately 640 m above sea level (which are more representative of the entire mixed layer).

Three of the photolysis reactions shown in Table 2 (Reactions 8, 14, and 23) vary with zenith angle in a manner similar to that of NO_2 photolysis. The photolytic rate constants for these reactions can be described by applying a single multiplication factor to the NO_2 photolytic constants. (For example, the multiplication factor for Reaction 8 is 0.053).

Seven of the reactions in Table 2 have photolysis rates that vary with zenith angle independently of NO_2 photolysis. The default ratios to NO_2 photolysis for four of these reactions (Reactions 9, 38, 39, and 45) are stored in OZIPM-4 and are shown in Table 4. A multiplication factor of 1.0 is entered into the rate constant slot of the reaction lines for these reactions.

Two of the species shown in Table 2 (OPEN and MGLY) are expected to photolyze with a zenith-angle dependence similar to that of formaldehyde photolysis to radicals (Reaction 38); H_2O_2 has a zenith-angle dependency that is similar to the photolysis of formaldehyde to stable products (Reaction 39). We therefore use the zenith-angle-dependent ratios given in Table 4 as default values for these reactions and multiply the resulting rates by the factors given in Table 2. If new rates other than those recommended in Table 4 are used, the factors given in Table 2 may have to be recalculated to maintain the same absolute rate constant.

4.3 DEFAULT VOC AND NMOC REACTIVITIES

The organic species in the CBM-4 mechanism (see Table 1) are the same as those found in the CBM-3 mechanism (Killus and Whitten, 1984; EPA, 1984), except that CARB (from the CBM-3) is divided into FORM and ALD2, ARO (from the CBM-3) is divided into TOL and XYL and ISOP is added. Therefore, many of the procedures described by EPA (1984) for the use of the CBM-3 in EKMA apply to the CBM-4 mechanism. Table 5 shows the recommended transported NMOC concentrations in the surface layer and aloft along with the default carbon fractions associated with the transported NMOC. Since OZIPM-4 does not contain any default concentrations for transported NMOC and aloft NMOC, it is recommended that the concentrations shown in Table 5 be used with CBM-4 when no specific measurements are available. Table 6 contains the default composition for the 0600-0900 NMOC mix and VOC emissions.

Reactivities of NMOC in numerous cities have been computed based upon K_{OH} values. K_{OH} values are rate constants which give a measure of the reactivity of a class of compounds with OH radicals. The weighted sum of these K_{OH} values gives an estimate of the overall reactivity of the NMOC mix.

TABLE 2. CBM-4 Photolysis Reactions

Reaction Number	Multiplication Reaction	Photolysis Rate
1	$NO_2 + h\ v \rightarrow NO + O$	See Table 3
8	$O_3 + h\ v \rightarrow O(^3P)$	$0.053 \times k_1$
9	$O_3 + h\ v \rightarrow O(^1D)$	See Table 4
14	$NO_3 + h\ v \rightarrow 0.89\ NO_2 + 0.89O$ $(^3P) + 0.11\ NO$	$33.9 \times k_1$
23	$HNO_2 + h\ v \rightarrow NO + OH$	$0.1975 \times k_1$
34	$H_2O_2 + h\ v \rightarrow 2OH$	$0.189 \times k_{39}$
38	$FORM + h\ v \rightarrow 2HO_2 + CO$	See Table 4
39	$FORM + h\ v \rightarrow CO$	See Table 4
45	$ALD2 + h\ v \rightarrow XO_2 + 2HO_2 + CO + FORM$	See Table 4
69	$OPEN + h\ v \rightarrow C_2O_3 + HO_2 + CO$	$8.40 \times k_{38}$
74	$MGLY + h\ v \rightarrow C_2O_3 + HO_2 + CO$	$8.96 \times k_{38}$

TABLE 3. NO_2 PHOTOLYSIS RATE CONSTANTS STORED IN OZIPM-4

Zenith Angle	Rate Constant*
0	0.5893
10	0.5851
20	0.5713
30	0.5470
40	0.5093
50	0.4537
60	0.3740
70	0.2578
78	0.1341
86	0.0242

*Units are min^{-1}

TABLE 4. PHOTOLYSIS REACTION RATE RATIOS STORED IN THE OZIPM-4[1]

Zenith Angle	ALD2 + h v → XO2 + 2HO2 + CO + FORM	FORM + h v → CO [2]	FORM + h v → 2HO2 + CO	O_3 + h v → O ^{1D}
0	5.89E-4	5.75E-3	3.70E-3	4.61E-3
10	5.78E-4	5.73E-3	3.66E-3	4.48E-3
20	5.50E-4	5.67E-3	3.56E-3	4.13E-3
30	5.03E-4	5.54E-3	3.40E-3	3.59E-3
40	4.36E-4	5.35E-3	3.14E-3	2.87E-3
50	3.55E-4	5.08E-3	2.80E-3	2.08E-3
60	2.57E-4	4.63E-3	2.33E-3	1.24E-3
70	1.59E-4	4.01E-3	1.74E-3	5.43E-4
78	8.95E-5	3.48E-3	1.28E-3	2.24E-4
86	8.26E-5	5.25E-3	1.78E-3	1.24E-4

Source: Jeffries and Sexton (1987)

[1] Ratios are relative to NO_2 photolysis. Rate constants are determined by multiplying the ratio by k_{NO_2}.

[2] These ratios, multiplied by the factor in Table 4-3 are also used for H_2O_2.

[3] These ratios, multiplied by the factors in Table 4-3, are also used for MGLY and OPEN.

The K_{OH} value for an NMOC mix can be determined using the following equation:

$$\overline{K_{OH}} = \text{PAR} * 1203 + \text{ETH} * 5960 + \text{OLE} * 21000 + \text{ALD2} * 12000 + \text{TOL} * 1307 + \text{XYL} * 4525 + \text{FORM} * 15000 + \text{ISOP} * 28400$$

Where: $\overline{K_{OH}}$ is the average K_{OH} value for the NMOC mix, PAR is the fraction of the mix considered paraffin (based upon the CBM-4 splits).

A typical city is expected to have an average K_{OH} value that falls between 2700 and 3600 min^{-1}. If the computed K_{OH} value, based upon a city-specific NMOC distribution, does not fall within this range, the process of determining the city-specific distribution should first be redone to check for errors. If no errors are found, the default reactivity should be utilized.

Requests to use reactivities other than the default must be reviewed and approved by the appropriate Regional Office in cooperation with the Model Clearinghouse.

4.4 SELECTING A USER-SPECIFIED ORGANIC REACTIVITY

If 0600-0900 ambient organic measurements are available, they may be used to calculate organic reactivity rather than using the default carbon fractions that are stored in OZIPM-4. Table 7 shows how to determine the CBM-4 fractions from 0600-0900 a.m. ambient data reported in ppmC.

The following paragraphs describe step-by-step how the organic reactivity is defined based on the ambient measurements shown in Table 7. Before we discuss these procedures, we note that, in general, ambient measurements are reported in the following units:

ppm (parts per million)

pphm (parts per hundred million)

TABLE 5. DEFAULT NMOC FRACTIONS USED IN OZIPM-4

	Carbon Fraction	
Species	Transported Surface Layer	Aloft Layer
ETH	*	0.034
OLE	*	0.020
ALD2	*	0.037
FORM	*	0.070
TOL	*	0.042
XYL	*	0.026
PAR	*	0.498
ISOP	*	0.000
NR	*	0.273
Total NMOC (ppmC)	*	0.030

*Assume to be zero.

TABLE 6. DEFAULT COMPOSITION FOR INITIAL NMOC MIX AND VOC EMISSIONS

Bond Type	Default Value
ETH	0.037
OLE	0.035
ALD2	0.052
FORM	0.021
TOL	0.089
XYL	0.117
PAR	0.564
ISOP	0.000
NR	0.085

*Fractional values (i.e., 3.7 percent of the carbon in a measured NMOC concentration is assumed to be Ethylene)

TABLE 7. CARBON BOND SPLITS FOR LOS ANGELES AMBIENT MEASUREMENTS*

Compound	ppmC	Carbon Number	ppm		OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
Ethane	.098	2	.049			.0196						.0784
Ethylene	.086	2	.943								.043	
Acetylene	.076	2	.038			.038						.038
Propane	.111	3	.037			.0555						.0555
Propene	.026	3	.0087		.0087	.0087						
Isobutane	.048	4	.012			.048						
Butane	.148	4	.037			.148						
1-Butene	.006	4	.0015		.0015	.003						
Isobutene	.012	4	.003			.003			.003	.003		
Isopentane	.221	5	.0043			.221						
Pentane	.081	5	.0162			.081						
Cyclopentane	.013	5	.0026			.013						
1-Pentene	.020	5	.004		.004	012						
2-Methylbutene	.004	5	.0008		.0008	.0004						
2,3-Dimethylbutane**	005	6	.0008			.005						
2-Methylpentane	.066	6	.0110			.066						
3-Methylpentane	.060	6	.0100			.060						
1-Hexene	.010	6	.0017		.0017	.0068						
N-Hexane	.060	6	.0100			.060						
Cyclohexane***	.064	6	.0107			.064						
2,2,3-Trimethylbutane	.054	7	.0077			.054						
Benzene	.049	6	.0082			.0082						.0410
2-Methylhexane	.048	7	.0069			.048						
3-Methylhexane	.044	7	.0063			.044						
1-Heptene	.031	7	.0044		.0044	.0220						
Heptane	.030	7	.0043			.030						
Methylcyclohexane	.026	7	.0037			.026						
2,2,3 &2,3,3-Trimethylpentane	.015	8	.0019			.015						
2,2,4-Trimethylpentane	.020	8	.0025			.020						
Toluene	.140	7	.020				.020					
1-Methylcyclohexene	.033	7	.0047		.0047	.023						

TABLE 7 (CONTINUED)

Compound	ppmC	Carbon Number	ppm		OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
2,2,5-Trimethylhexane	.009	9	.0010			.009						
N-Octane	.017	8	.0021			.017						
Ethylbenzene	.033	8	.0041			.0041	.0041					
P,M-Xylenes	.112	8	.014					.014				
O-Xylenes	.048	8	.0060					.006				
N-Nonane	.012	9	.0013			.012						
Propylbenzene	.009	9	.0010			.002	.001					
Sec-butylbenzene	.050	10	.0050			.015	005					
N-Decane	.011	10	.0011			.011						
N-Undecane	.011	11	.0010			.011						
N-Dodecane	.004	12	.0003			.004						
TOTAL	2.021				.026	1.290	.030	.202	.003	.003	.043	.212

*Source of hydrocarbon data: Calvert (1976)

**Incorrectly reported as 2,2 dimethylbutene by Calvert (1976).

***Incorrectly reported as cyclohexene by Calvert (1976).

Table 7b

Compound	NMOC ppm	Carbon Number ****	NMOC ppmC	Carbon Fraction	Adj Carbon Fraction	Compound	Final** Carbon Fraction
OLE	.026	2	.052	.026	.026	OLE	.025
PAR	1.290	1	1.290	.638	.638	PAR	.608
TOL	.030	7	.21	.104	.104	TOL	.099
XYL	.020	8	.160	.079	.079	XYL	.075
FORM	.003	1	.003	.001	.021	FORM	.020
ALD2	.003	2	.006	.003	.033	ALD2	.031
ETH	.043	2	.086	.043	.043	ETH	.041
NR	.213	1	.213	.105	.105	NR	.100

**** - From Table 1

** - Totals adjusted to 1.00

ppb (parts per billion)

$\mu g/m^3$ (micrograms per cubic meter)

In some cases, the organic compounds may be expressed in the above units either as a molecular total or as a carbon total (i.e., the actual molecular weight or the molecular weight of carbon is used). In general, chemical mechanisms are based on molecular reactions or the number of molecules involved. The first three units presented above are in the units necessary for most chemical mechanisms. The fourth unit is a mass unit and must be converted to molecular units. The following equation is used to convert mass units to molecular units:

$$C_{ppm} = \frac{0.0244}{MW} \times C_{\mu g/m}{}^{3}$$

where MW is the molecular weight in units of g/mole of the organic compound. Molecular weights for many compound are given in Table B-1. The conversion factor, 0.0244, is based on the perfect gas law at 25°C and standard pressure. To obtain molecular units as carbon, one needs to multiply by the number of carbons found in the organic compound. (Also shown in Table B-1).

Table 7 shows ambient organic compound measurements in the Los Angeles area (Calvert, 1976). The measurements are reported in molar units (ppmC in this case). To obtain the carbon bond reactivity, one must convert the readings from ppmC to ppm. This is done by dividing the concentration in ppmC by the carbon number for the compound. Once the concentrations are in ppm, one must assign the individual carbon atoms of each organic compound to the appropriate carbon bond group according to Table B-2 in Appendix B. Table B-2 shows the assignment for each carbon atom from the molecular compound to the carbon bond groups. For example, the organic compound C_3H_6 (Propene) shown in Table 7 comprises one OLE and one PAR. Thus, of the three carbon atoms of propene, two are assigned to OLE (because each OLE group contains two carbons), and one is assigned to PAR. To calculate the concentrations of OLE and PAR from propene, we multiply the number of each bond group by the concentration of propene (in ppm). Thus, the propene concentration of 0.0087 ppm produces 0.0087 ppm of OLE and 0.0087 ppm of PAR. As another example, Appendix B shows that benzene (C_6H_6) consists of five NR and one PAR. Applying the above procedures, we obtain 0.041 ppm of NR and 0.0082 ppm PAR.

This procedure is followed for all the organic compounds identified in Table 7. The carbon bond concentrations are summed as shown in Table 7b. The OZIPM-4 requires all organic fractions to be on a "per carbon" basis. Thus, the concentrations for each carbon bond group are multiplied by the appropriate number of carbons reported in Table 2. These values are then divided by the total NMOC (2.021 ppmC) to obtain carbon fractions.

In the example presented in this section, only surrogate carbonyls could be included in the speciations because carbonyl compounds per se (aldehydes and ketones) could not be detected by the instrumentation used. Carbonyl compounds were undeniably present, however, and they are significant contributors to smog chemistry. Therefore, some estimates of carbonyl emissions must be made. Investigations by Killus and Whitten (1984) show that an estimated 5 percent of the total organics are carbonyls. Of the 5 percent, 60 percent is ALD2 and 40 percent is FORM. Thus, for those cases in which there are no measured carbonyls, we must add 5 percent carbonyls (3 percent ALD2 and 2 percent FORM) to the total organics. The carbon fractions adjusted for the carbonyls are shown in the fifth column of Table 7b. Please note that the individual carbon fractions must be adjusted so that they total 1.00 and not 1.05. For this example, the numbers shown in Column 5 of Table 7b would be input into the OZIPM-4 program if the user chose not to utilize OZIPM-4's default assumptions concerning reactivity.

5.0 USER'S GUIDE

This chapter describes the format of the input data, the types of errors and warning messages that can occur, and some special problems to be considered in the installation of the OZIPM-4 program on a specific facility.

The system structure of OZIPM-4 is shown in Figure 4. The program retrieves card-image input, and produces line printer output. Two optional output files may also be generated by the user. The first is an output file that contains the data needed to produce an isopleth diagram on an off-line plotter. The second file contains information on the change in ozone as a function of VOC emission reduction that is produced by the EKMA routine.

A simulation section controls the individual model simulations, and an interpolation and plotting section controls the generation of isopleth diagrams. OZIPM-4 also contains a section to directly estimate the VOC control calculations; the EKMA routine.

5.1 FORMAT OF INPUT DATA

The options in OZIPM-4, which were discussed in Section 3, are listed in alphabetical order in Table 8.* For each option, the locations of the different parameters on the appropriate lines are shown. The order of the OZIPM options in the input file is not important except for the ISOPLETH, EKMA, and CALCULATE options. Any options to be activated for simulations must precede these three options. One other exception is that the TIME option must precede the DILUTION option. Consequently, the following order is recommended. Options used to input city-specific information (PLACE, TIME, DILUTION, TEMPERATURE, EMISSIONS, CREDIT, REACTIVITY, TRANSPORT, BIOGENICS and WATER, etc.) should be

---

*For convenience, Table 8 appears at the end of this section.

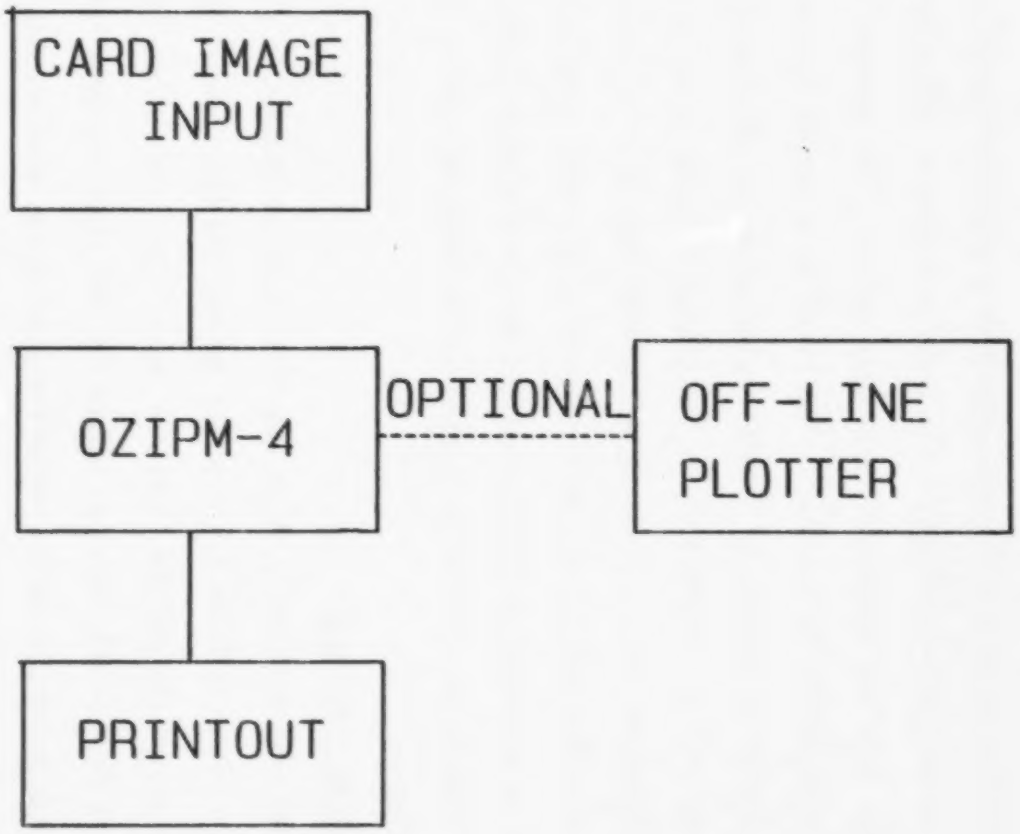
CARD IMAGE
INPUT
OZIPM-4
OPTIONAL
OFF-LINE
PLOTTER
PRINTOUT

FIGURE 4 SCHEMATIC OF OZIPM-4 SYSTEM

listed first. The next group of options affects some of the operational aspects of OZIPM (ACCURACY, ALREADY, PLOT, and SPECIES). The options that actually initiate simulations follow (CALCULATE, EKMA, and ISOPLETH). The last line of any input set must be a blank line.

As shown in Table 8, all four-letter code words (e.g., TITL, PLAC, etc.) that activate an option must begin in Column 1. Each line containing such a code word has up to six numeric fields, each ten spaces wide, beginning in Column 11. An entry can be made anywhere in a field, but a decimal point must always be used, even with integer values. Additional data lines are associated with some options. These lines must follow the option line in the order specified in Table 8. For example, the line containing the title must immediately follow the line with the code word TITL. Data lines that do not begin with code words can contain up to seven 10-column fields beginning in Column 1. Similar to the numeric fields on lines with code words, entries may be made anywhere in the field provided a decimal is used.

As previously described, most parameters have associated default values. These are indicated by DF in Table 8. If no entry is made in a numeric field, the default value will be assumed. For example, if the only entry made on the PLACE line is in the first numeric field, the default value of 118.25 will be assumed for the second numeric field, 7.0 for the third, etc.

5.2 PROGRAM-GENERATED ERROR MESSAGES

This section discusses potential output error messages produced by OZIPM-4. Two types of error messages can be generated:

(1) Fatal error messages--messages caused by problems that immediately halt any further computation.

(2) Nonfatal error messages--messages caused by problems that do not cause an immediate halt in computation.

These types of messages are discussed next.

5.2.1 Fatal Error Messages

Seven fatal error messages can occur during OZIPM runs. Five of these occur because the integration scheme cannot proceed further. Descriptions of each message are included here:

THE LOWEST OZONE LINE CANNOT BE PLOTTED; INCREASE THE MAXIMUM HC AND NO_x VALUES

If the concentration of ozone predicted from the maximum NMOC and NO_x concentrations (listed on the ISOPLETH line, or NMOC = 2.0, NO_x = 0.14 by default) is less than the lowest ozone isopleth line to be plotted, the program will stop. The user can fix this problem either by increasing the maximum NMOC or NO_x concentrations or by reducing the concentrations at which ozone isopleths are to be plotted.

NO LINES CAN BE PLOTTED; BACKGROUND ONLY PRODUCES TOO MUCH OZONE ________ PPM

This message is the opposite of the previous message. If the amount of ozone predicted at NMOC and NO_x concentrations of 0.0 is greater than the highest ozone isopleth line desired, the program will stop.

The following error messages all stem from problems encountered in the integration scheme routines:

PROBLEM APPEARS UNSOLVABLE WITH GIVEN INPUT

INTEGRATION HALTED BY DRIVER AT T = ___, EPS TOO SMALL TO BE ATTAINED FOR THE MACHINE PRECISION

KFLAG = -2 FROM INTEGRATOR AT T = _____, H = _____ THE REQUESTED ERROR IS SMALLER THAN CAN BE HANDLED

KFLAG = -3 FROM INTEGRATOR AT T = _____ CORRECTOR CONVERGENCE COULD NOT BE ACHIEVED
ILLEGAL INPUT..EPS.LE.0

If any of these messages occur, the user should try the following procedures:

Check input to be sure all data are correct (e.g., check NMOC and NO_x values on a CALCULATE option, check for negative error tolerance on the ACCU option line, and so on).

Raise the value of the error tolerance, if necessary, by adjusting the value in the third field of the ACCURACY option.

Redefine the density of simulations (e.g., change the maximum NMOC or NO_x concentrations).

As a last resort, alter the simulation conditions slightly (e.g., change emissions, dilution, etc.).

5.2.2 Nonfatal Error Messages

One nonfatal error message can occur in OZIPM-4 runs. The user may wish to redefine the situation (i.e., the limits of the diagram) or to check the input data.

THE OPTIONS INSTRUCTION___CANNOT BE PROCESSED

If this message occurs, the user should check for an error in the input data.

5.3 COMPUTER CONSIDERATIONS

The OZIPM-4 program consists of one main program and 55 subprograms. It requires about 30,000 16-BIT words of core in a PRIME 750 computer system. Typical run times with the ISOPLETH option on the IBM 3090 computer are usually less than 5 minutes. Complete listings of the source code are shown in Volume 2. Also included in OZIPM-4 are five calls to CALCOMP subroutines.

The following paragraphs discuss special language considerations, use of CALCOMP routines, and computer control language.

5.3.1 Language Considerations

Although OZIPM-4 has been written to conform with ANSI standard FORTRAN language, certain features of the code in OZIPM-4 are not compatible on all computer systems. The variable UROUND in BLOCK DATA should be set to the round-off error associated with each computer system. Currently, UROUND is set to the round-off error of 2.4×10^{-7} associated with a PRIME 750 computer system. To reset UROUND, line B55 in the BLOCK DATA routine should be changed as follows:

```
DATA    UROUND/user's round-off error/
```

UROUND is calculated from the number of significant digits (N) used for the mantissa of a floating point constant:

$$\text{UROUND} = 2^{-N}.$$

For the PRIME 750 computer, each word contains 32 BITs, of which 22 are used for the mantissa. Thus, 2^{-22} is equal to approximately 2.4×10^{-7}. This is the value currently set in OZIPM-4.

Another variable in OZIPM-4 that is machine-dependent is EXPMAX, which is found in subroutines CURV1 and KURV1. This variable represents the maximum possible value for the exponent of e. For the PRIME computer, the range of the real constants is from 10^{-38} to 10^{38}. Hence, the maximum value for the exponent of e is

$$e^{\text{EXPMAX}} = 10^{38},$$

i.e., EXPMAX is 87.4 for the PRIME computer, the value currently set in OZIPM-4. To reset EXPMAX, the user must change line B55 in BLOCK DATA accordingly:

```
DATA EXPMAX/user's maximum exponent/
```

The OZIPM-4 prints the input file on the output file so that users can easily see any problems with the input file. To do this, the input file (FORTRAN unit 5) must be rewound. Some computer systems do not allow a rewind option on the input file. If this is the case, lines A125-A136 in the MAIN routine should be taken out. Some computer systems do not allow arguments to be in a mixed mode (i.e., a REAL variable declared as INTEGER in separate subroutines). If this is the case, line AG13 in subroutine NSSFAC must be modified to be REAL instead of INTEGER.

5.3.2 Use of CALCOMP Routines

The CALCOMP routines required by OZIPM-4 are

```
Subroutine PLOT (XX,YY,IX)
     PLOTS (XX,UU,IX)
     SYMBOL (XX,YY,HT,ITX,ANG,NCH)
     NUMBER (XX,YY,TC,FPN,ANG,NDEC)
     NEWPEN (IPEN)
```

For users without access to these CALCOMP routines, dummy routines may be needed to run OZIPM-4. To generate the dummy routines, the user must have the following lines for each of these CALCOMP routines:

```
SUBROUTINE_________(argument list)

RETURN

END
```

For users with access to standard CALCOMP routines, no modifications to OZIPM-4 are required. Users should check to ensure that the five routines in their system have the same names as those given above.

Control Language- Since the job control language necessary to run OZIPM-4 is different for each computer system, only the files required by the program are presented in this section. Table 9 lists the files and the FORTRAN file unit numbers used by OZIPM-4.

TABLE 8. INPUT FORMAT FOR OZIPM-4 OPTIONS

Option	Line No.	Column	Contents
ACCURACY	Increase or reduce the mathematical accuracy of the isopleth diagram by using more or less accurate interpolation, etc.		
	1	1-4	ACCU
		11-30	Not read
		31-40	Error tolerance in the numerical integration routine, from 0.1 to 0.00001; (DF = 0.003)
		41-50	Tension factor for hyperbolic spline functions used in first stage of interpolation from 0.001 to 50.; (DF = 1)
		51-60	Tension factor for hyperbolic spline functions used in plotting isopleth lines (high tensions lead to straight lines drawn between the points obtained from the first stage), from 0.001 to 50.; (DF = 1)
		61-70	If any nonzero value is entered in this field, simulations will terminate after any ozone maximum; no entry produces results over the total simulation period

TABLE 8 (Continued)

Option	Line No.	Column	Contents
ALREADY*	Include results from a previous run.		
	1	1-4	ALRE
		11-20	Number of previous simulations to be input If the number is positive, then read the following lines. If the number is negative, then read previous simulation results from an external file
	2	1-10	NMOC concentration
		11-20	NO_x concentration
		21-30	Maximum 1-hour average ozone concentration, ppm
		31-40 41-50 51-60 61-70	Maximum 1-hour average concentrations (ppm) of any other species for which isopleths are to be constructed. These values are optional depending on the number of species declared on the SPECIES line. (Must be in the same order as listed on the SPECIES line.)

*Can only be used with the ISOPLETH options.

TABLE 8 (Continued)

Option	Line No.	Column	Contents
BIOGENICS	Allow for post-0800 biogenic emissions. If the BIOG option is not used, defaults are no post-0800 biogenic emissions, and no transported surface concentrations and aloft concentrations of biogenics.		
	1	1-4	BIOG
		11-20	Number of emission hours. Must be equal to number of hours set in EMIS or MASS options. (Expressed as a negative number)
		21-30	Enter the number of biogenic species (DF=0, max=5).
		31-40	Initial mixing height. Used to convert mass units in kg/km^2 to ppm. Units must be in meters.
	The next set of lines are repeated for each biogenic species.		
	2+	1-4	Species name. (Note: If Isoprene is used then the default name should be ISOP).
		11-20	Flag to treat biogenic species as a specific molecular species or as Carbon Bond IV species (Enter a nonzero value in order to treat the biogenic species as CB-IV species). Note: Isoprene is the only biogenic species currently treated specifically in the CB-IV mechanism.
		21-30	Present-day concentration transported in the surface layer (DF=0)
		31-40	Present-day concentration transported aloft (DF = 0.0)
		41-50[**]	Percent change in biogenic emissions for the future year

---

[**] Not used with CALC and ISOP options.

TABLE 8 (Continued)

Option	Line No.	Column	Contents
		51-60**	Future-year concentration transported in the surface layer (DF=0)
		61-70**	Future-year concentration transported aloft (DF = 0.0)
		71-80	Not read
	3+	1-10	Species molecular weight (Units of gm/moles)
	4+ (optional)	1-10 11-20	If a nonzero value is entered on columns of line 2, the species profiles by bond group of the biogenic species is entered here.
		11-20	The species profiles should be in the following order: ETH, OLE, ALD2, FORM, TOL, XYL, PAR, and NR.
		. .	
		61-70	Continue on next line (if necessary).
		71-80	Not read
	5+	1-10	Present-day hourly biogenic emissions (kg/km^2)
		11-20	(continue on next line if necessary)
		. . .	
		61-70	

**Not used with CALC and ISOP option

TABLE 8 (Continued)

Option	Line No.	Column	Contents
CALCULATE	Perform a single simulation with the initial NMOC and NO$_x$ concentrations specified on this line.		
	1	1-4	CALC
		11-20	NMOC concentration
		21-30	NO$_x$ concentration
		31-40	Information option; entry of any positive value will result in printing of the computed concentrations of all species, the rate of change of all species, reaction rates, etc. Photolysis constants are also printed
		41-50	Time (in minutes) from the beginning of the simulation at which computed concentrations of all species in the kinetic mechanism are to be printed; (DF = 60)
		51-60	Time step (in minutes) for subsequent printing of concentrations; (DF = 60)

TABLE 8 (Continued)

Option	Line No.	Column	Contents
CREDIT	Allow for post-8 a.m. CO emissions in EKMA calculations. Defaults are no post-8 a.m. CO emissions, 1.2 ppm CO for the 6-9 a.m. measurement and 0.5 ppm CO aloft.		
	1	1-4	CRED
		11-20	Enter a negative number to defeat use of this option in multiple runs.
		21-30	Number of emission hours entered as a negative number. Must be equal to the number of hours set in MASS option.
		31-40	Initial mixing height.
	2	1-10	Species names. CO is the only name allowed.
		11-20	6-9 a.m. present day CO concentration
		21-30	Not read
		31-40	Present day CO transported aloft (DF = 0.5)
		41-50	Percent change in CO emissions and 6-9 a.m. concentration for the future year
		51-60	Not read
		61-70	Future year CO transported aloft
	3	1-10	Present hourly emissions of CO
		11-20...	in kg/km^2

TABLE 8 (Continued)

Option	Line No.	Column	Contents
DILUTION	Read site-specific information on initial and final mixing heights. Dilution is calculated using the characteristic curve.		
	1	1-4	DILU
		11-20	Initial mixing height, Z1, meters (DF = 510 m)
		21-30	Final mixing height, Z2, in same units as initial mixing height (DF = 630 m)
		31-40	Starting time of mixing height change (2400 hour) (DF = 0800)
		41-50	Ending time of mixing height change (2400 hour) (DF = 1500)
		51-60	Dilution rate in percent per hour before and after the mixing height change (DF = 0)
		61-80	Not read

TABLE 8 (Continued)

Option	Line No.	Column	Contents
EKMA	Used to perform a VOC emission requirement calculation.		
	1	1-4	EKMA
		11-20	Base-case ozone concentration, ppm
		21-30	NMOC/NO_x ratio (If the value is negative, the base-year NMOC and NO_x levels have been determined in a previous simulation and are entered on line 3. Future-year calculations are performed based on the base-year NMOC and NO_x levels.)
		31-40	Percentage change in NO_x emissions; positive number for increase, negative number for decrease (DF = 0)
		41-50	Change in transport option indicator; if nonzero, input line 2 is required (DF = 0)
		51-60	Option to generate report of change in ozone as a function of change in VOC emissions; if 1., generate tabular report; if 2., generate tabular report and write results on file. (DF = 0., i.e., no report or file generated)
		61-70	Flag to do a calculation at a specified NMOC level. The NMOC level is expressed as a percent change from the base year level. The value is placed on line 2, Columns 61-70. Any nonzero value may be used as the flag.

TABLE 8 (Continued)

Option	Line No.	Column	Contents
EKMA	The next line is included only if a nonzero entry is specified on line 1 for the transport option (41-50) and/or the flag option (61-70)		
	2 (optional)	1-10	Concentration of ozone transported in surface layer for post-control conditions, ppm; (DF = base-case level). A negative value activates the use of the future ozone transport estimate curves shown in Figure 3. (A value less than -100 activates the use of the dashed line shown in Figure 3.)
		11-20	Concentration of ozone transported aloft for post-control conditions, ppm; (DF = base-case level). A negative value activates the use of the future ozone transport estimate curves shown in Figure 3. (A value less than -100 activates the use of the dashed line shown in Figure 3.)
		21-30	Concentration of NMOC transported in the surface layer for postcontrol conditions, ppmC; (DF = base-case level).
		31-40	Concentration of NMOC transported aloft for post-control conditions, ppmC; (DF = base-case level).
		41-50	Concentration of NO_x transported in surface layer for post-control conditions, ppm; (DF = base-case level)
		51-60	Concentration of NO_x transported aloft for post-control conditions, ppm; (DF = base-case level)

TABLE 8 (Continued)

Option	Line No.	Column	Contents
The following line must be included.			
EKMA	3	1-10	Measured 6-9 a.m. NMOC (value used in emission density calculations) (DF = 0)
		11-20	Measured 6-9 a.m. NO_x (value used in emission density calculations) (DF = 0)
		21-30	Calculated NMOC that yields base case O_3. Declared if a negative NMOC/NO_x ratio is entered on line 1(DF = 0)
		31-40	Calculated NO_x that yields base case O_3. Declared if a negative NMOC/NO_x ratio is entered on line 1 (DF = 0)
		41-50	Change in NMOC level (percent) for specific calculation after the base-year ozone is estimated. (Used only if column 61-70 of line 1 is nonzero.)

TABLE 8 (Continued)

Option	Line No.	Column	Contents
ISOPLETH	Construct isopleth diagrams for O_3 and other species according to the input parameters. Default isopleths for O_3 are 0.08, 0.12, 0.16, 0.20, 0.24, 0.28, 0.30, 0.32, 0.34, 0.36, and 0.40 ppm.		
	1	1-4	ISOP
		11-20	Maximum NMOC concentration on abscissa of isopleth diagram; (DF = 2.0 ppmC)
		21-30	Maximum NO_x concentration on ordinate of isopleth diagram; (DF = 0.28 ppm)
		31-40	Number of ozone isopleths to be drawn, from 1. to 20.; (DF = 11)
		41-50	Any nonzero value will activate the printing of solar noon and the time of the center of the maximum 1-hour average ozone concentration for each simulation
		51-60	Not read
		61-70	Number of species to plot. This number corresponds to the number of species entered on the PLOT option.
	2 (optional)	1-10	Ozone concentration of 1st isopleth, ppm
		11-20	Ozone concentration of 2nd isopleth, ppm
		21-30	Ozone concentration of 3rd isopleth, ppm
		31-40	Ozone concentration of 4th isopleth, ppm
		41-50	Ozone concentration of 5th isopleth, ppm
		51-60	Ozone concentration of 6th isopleth, ppm
		61-70	Ozone concentration of 7th isopleth, ppm

TABLE 8 (Continued)

Option	Line No.	Column	Contents
	3 (optional)	1-10 . . .	Ozone concentration of 8th isopleth, ppm
		61-70	Ozone concentration of 14th isopleth, ppm
	4 (optional)	1-10 . . .	Ozone concentration of 15th isopleth, ppm
		51-60	Ozone concentration of 20th isopleth, ppm

TABLE 8 (Continued)

Option	Line No.	Column	Contents
MASSEMISS			Used to supply mass emission densities through which post-0800 emission fractions are computed.
	1	1-4	MASS
		11-20	Number of hours of emissions (max = 24.)(expressed as a negative number)
		21-30	Initial NMOC concentration (used to compute NMOC emission fractions, ppmC)
		31-40	Initial NO_x concentration (used to compute NO_x emission fractions, ppm)
		41-50	Mixing height at start of simulation, in meters
			The next line is repeated if more than 7 hours of emissions are specified. The number of entries must equal the number of hours specified on line 1.
	2	1-10	VOC emission density for hour 1, kg/km^2
		11-20	VOC emission density for hour 2, kg/km^2
		.	
		.	
		.	
		61-70	VOC emission density for hour 7, kg/km^2
			The next line is repeated if more than 7 hours of emissions are specified. The number of entries must equal the number of hours specified on line 1.
	3	1-10	NO_x emission density for hour 1, kg/km^2
		11-20	NO_x emission density for hour 2, kg/km^2
		.	
		.	
		.	
		61-70	NO_x emission density for hour 7, kg/km^2

TABLE 8 (Continued)

Option	Line No.	Column	Contents
PLACE	Input city-specific information on light intensity. Default values correspond to Los Angeles on June 21, 1986.		
	1	1-4	PLAC
		11-20	Latitude, in decimal degrees north of the equator (DF = 34.058)
		21-30	Longitude, in decimal degrees west of Greenwich meridian (DF = 118.250)
		31-40	The time zone, in hours from Greenwich mean time (DF = 7.0)
		41-50	The year (DF = 1986)
		51-60	The month of year (DF = 6)
		61-70	The numerical day of month (DF = 21)
	2 (optional)	1-24	The name of the place can be entered anywhere in columns 1-24. Include this line only if a new value is entered for the latitude or longitude on the previous line.

TABLE 8 (Continued)

Option	Line No.	Column	Contents
PLOT	Activates the drawing of the isopleth diagram on an off-line plotter.		
	1	1-4	PLOT
		11-20	Scaling factor for the location of labels for each ozone isopleth. The value should be between 0.1 and 0.8.; (DF = 0.6)
		21-30	If nonzero, a grid is overlaid onto the diagram. If the value is positive and nonzero, a grid is overlaid on the diagram using a different color pen (if available) If the value is negative, a grid with line of different patterns (e.g., dot-dash) is overlaid on the plot. The absolute value of this number corresponds to different patterns and textures
		31-40	Length (in inches) of the abscissa (NMOC scale) of the isopleth diagram; (DF = 8.5)
		41-50	Length (in inches) of the ordinate (NO_x scale) of the isopleth diagram; (DF = 5.95)
		51-60	Size (in inches) of the numbers to be printed on the axes and of the characters in the title; (DF = 0.10)
		61-70	The size (in inches) of the labels on the ozone isopleths and the division marks on the axis; (DF = 0.07)

TABLE 8 (Continued)

Option	Line No.	Column	Contents
REACTIVITY*	Contains site-specific information on organic reactivity and NO_2/NO_x ratio for the initial 6-9 AM mix and the VOC and NO_x emissions.		
	1	1-4	REACT
		5-10	Not read
		11-20	The number of primary organic species in the chemical mechanism (DF=9)
		21-30	The NO_2/NO_x fraction
	2	1-10 61-70	The reactivity for each of the organic species (up to 7 on a line) represented as the fractions of total NMOC. Continue on next line (if necessary)
		71-80	Not read

---

*If the REACTIVITY option is not used, the default fractions are those shown in Table 5, Section 4.

TABLE 8 (Continued)

Option	Line No.	Column	Contents
SPECIES	This option allows the user to plot isopleths for any species found in the kinetic mechanism or to plot concentration-time profiles for species besides 0, if the CALCULATE option is used.		
	1	1-4	SPEC
		11-20	Number of species to be plotted (DF = 1). Max = 5
		21-80	Not read
		1-4 11-14 21-24 31-34 41-44	The alphanumeric symbol of the species of interest; left-justified (DF = 03 [ozone])
		45-80	Not read

TABLE 8 (Continued)

Option	Line No.	Column	Contents
TEMPERATURE	A varying diurnal temperature profile may be used during the simulation with this option. Temperature values should be in units of degrees K. Values are read for the initial time and at the end of each hour. If there are n hours, there should be n+1 temperature values.		
	1	1-4	TEMP (DF = 303 K)
		11-20	Number of hours (n) of varying temperature (MAX = 24)
		21-30	Temperature at time t = 0
		31-40	Temperature at time t = 1 hr
		41-50	Temperature at time t = 2 hr
		51-60	Temperature at time t = 3 hr
		61-70	Temperature at time t = 4 hr
		71-80	Not read
			If more than 4 hours of values, continue on next line
	2+ (optional)	1-10	Continuation of temperature values
		.	
		.	
		.	
		61-70	
		71-80	Not read

TABLE 8 (Continued)

Option	Line No.	Column	Contents
TIME	Reset starting and ending times for simulations with this option.		
	1	1-4	TIME
		5-10	Not read
		11-20	Starting time for simulations based on 24-hour clock (DF = 0800)
		21-30	Ending time for simulations (DF = 1800). Note: Maximum difference is 24 hours
		31-80	Not read

TABLE 8 (Continued)

Option	Line No.	Column	Contents
TITLE	Input a new title. If this option is not activated, the default title is "Standard Ozone Isopleth Conditions."		
	1	1-4	TITL
	2	1-72	The title can be placed anywhere in line between columns 1-72

TABLE 8 (Continued)

Option	Line No.	Column	Contents
TRANSPORT	Option for site-specific information on O_3, NO_2, NMOC transported in the surface layer and in the air aloft that is entrained as the mixing height rises. (If TRAN option is not used, concentration of transported species is 0.)		
	1	1-4	TRAN
		11-20	Transported ozone concentration in the surface layer (ppm)
		21-30	Ozone entrained from aloft (ppm)
		31-40	If nonzero and positive:* Transported NMOC in the surface layer (ppmC)
		41-50	If nonzero and positive:* Total NMOC entrained from aloft (ppmC)
		51-60	Transported NO_x in the surface layer (ppm)
		61-70	NO_x entrained from aloft (ppm)
		71-80	Not read
	2 (optional)	1-10	If a nonzero negative value is entered in columns 31-40 of the TRAN line, the total NMOC transported in the surface layer is entered here (ppmC).
		11-20	The fraction of the total NMOC for each of the organic species transported in the surface layer (should be in the following order: ETH, OLE, ALD2, FORM, TOL, TYL, PAR, ISOP, and NR.
		61-70	Continue on next line (if necessary)
		71-80	Not read

---

*The default carbon fractions for NMOC transport in the surface layer and for NMOC aloft are given in Table 5, Section 4.

TABLE 8 (Continued)

Option	Line No.	Column	Contents
TRANSPORT			
	3 (optional)	1-10	If a nonzero negative value is entered in columns 41-50 of the total NMOC entrained from aloft is entered here (ppmC)
		11-20 61-70	The fraction of the total NMOC entrained for each of the organic species entrained from aloft. Continue on next line (if necessary)
		71-80	Not read

TABLE 8 (Continued)

Option	Line No.	Column	Contents
WATER	Allows for varying water concentration profile. This option must follow the TEMPerature option. Information is entered regarding the number of hours with varying water concentrations, the hourly relative humidity, and the atmospheric pressure. The relative humidity values are read for the initial time and at the end of each hour. If there are n hours, there should be n+1 relative humidity values. If the WATE option is not used, the default water concentration is 20000 ppm.		
	1	1-4	WATE (DF = 20000 ppm)
		11-20	Number of hours of varying water concentrations. (MAX = 24)
		21-30	Enter the atmospheric pressure; units of inches of Hg. (DF=29.92 inches of Hg which is equal to 1 atm)
	2	1-10	Relative humidity (in percent) at time t = 0
		11-20	Relative humidity at time t = 1 hr
		21-30	Relative humidity at time t = 2 hr
		31-40	Relative humidity at time t = 3 hr
		41-50	Relative humidity at time t = 4 hr
		51-60	Relative humidity at time t = 5 hr
		61-70	Relative humidity at time t = 6 hr
		71-80	Not read
	3+ (optional)	1-10	Continuation of relative humidity values
		.	
		.	
		.	
		61-70	
		71-80	Not read

TABLE 8 (Continued)

Option	Line No.	Column	Contents
bbbb	A blank line must follow all input lines to terminate the program.		
	1	1-4	Blanks

TABLE 9. FILES USED BY OZIPM-4

File	FORTRAN Unit*	Read (R)/ Write (W)	Comment
Input file	5	R	The line input deck (line-image)
Output file →	6	W	The output of the OZIPM-4 results
ALREADY file	9	W	The results of each simulation on a diagram point are written to this file for later use
ALREADY file	8	R	File of results from a previous run used to continue an isopleth simulation or redo the isopleth
PLOT file (optional)	--	W	The file to which CALCOMP or offline plots are written. The file unit is dependent on the computer system
EKMA file (optional)	11	W	The file to which EKMA calculations are written when the range option is invoked

---

*Each of the unit numbers can be changed in the OZIPM-4 program bymodifying the following statement in the BLOCK DATA routine:

```
DATA IN/5/, IOUT/6/, IALN/9/, IALL/8/, IOZC/11/.
```

6.0 EXAMPLE OZIPM-4 RUNS

This chapter outlines five OZIPM-4 runs which cover the basic output options. First, a test case run will be discussed so that a prospective user may ensure that OZIPM-4 is functioning properly on the user's computer facilities. The subsequent sections deal with predicting peak ozone (CALC option), making a VOC control estimate without generating an isopleth diagram (EKMA option), and generating a base and future case isopleth diagram (ISOP option).

6.1 OZIPM-4/CB-4 TEST CASE

When dealing with a model and chemical mechanism as complex as OZIPM-4 and CB-4, special emphasis should be placed on ensuring that the program is operating correctly. The easiest way to check is by comparison with a test case. The input data for the test case has been kept simple in order to avoid the possibility of introducing errors that could be due to some of the other model inputs. Thus, before proceeding to city-specific simulations, replication of the test case simulation discussed here is recommended.

The input data required to generate the OZIPM-4 output for comparison with the test case are shown in Table 10.

The output that is generated by OZIPM-4 using the inputs in Table 10 is shown in Appendix C. Prospective users should find close agreement between their output and that shown. However, some discrepancies will likely occur as a result of differing computer systems. As a rule of thumb, predicted ozone concentrations should agree to the third decimal place.

TABLE 10. INPUT DATA FOR TEST CASE RUN

```
1     TITL
2     TEST CASE
3     CALC         1.0       .1
4
```

6.2 PREDICTION OF PEAK OZONE

Table 11 shows the input structure for a sample case in which a single simulation is to be conducted for the purpose of predicting peak ozone.

The output generated using this input stream is contained in Appendix D. Worthy of note is the fact that the predicted ozone concentrations are printed for each hour of the simulation period.

6.3 PERFORMING AN EKMA CALCULATION

In the past, ozone isopleth diagrams have been prepared in order to determine the initial NMOC and NO_x concentrations needed to reduce the daily maximum ozone concentration to the level of the NAAQS. The new recommended approach is to utilize the EKMA option to estimate a VOC control target. The option is quicker than the use of the ISOPLETH option.

Table 12 shows the input structure for a sample case in which the EKMA option is applied. The output generated by this example is contained in Appendix E.

6.4 GENERATING A BASE CASE DIAGRAM WITH THE ISOP OPTION

The example discussed in this section is a follow-on to the one just described. Suppose that, using the same model data, the goal is to generate an ozone isopleth diagram rather than to use the EKMA option. The ISOP option allows the user more flexibility concerning simulation of changes which occur concurrently with changes in VOC and NO_x. Ordinarily, two diagrams are needed. As described in EPA (1989), these must be superimposed so that controls needed to reduce current O_3 (base case diagram) to the 0.12 ppm (future case diagram) can be seen. The first diagram is presumed to represent

TABLE 11. EXAMPLE INPUTS FOR PREDICTING PEAK OZONE

```
TITL
EXAMPLE OF SINGLE CALCULATION
PLAC          38.629    90.206        6.     1988.        6.       21.
TEST CITY
DILO            250.     1700.        0.        0.        0.
TEMP             11.      294.      296.      299.      301.      304.
      305.      307.      308.      306.      305.      304.      302.
WATE             11.     29.95
       80.       75.       50.       45.       40.       35.       30.
       30.       30.       30.       35.       40.
TRAN              0.       .04        0.       .03        0.      .002
MASS            -11.       .80       .08      250.
      9.42      7.68      7.54      5.21      3.23      2.24      2.18
      1.75      1.72      2.10      1.12
      8.11      6.18      5.65      4.11      2.76      1.90      1.91
      1.60      1.42      1.78       .90
BIOG            -11.        2.      250.
ISOP              0.     .0001        0.        0.     .0001        0.
     68.12
        0.        0.        .1        .3        .8       1.0       1.5
       1.3       1.0        .8        .6
APIN              1.     .0001        0.        0.     .0001        0.
    136.24
        0.        .5       1.5        0.        0.        0.        6.
        0.
        0.        0.        .2        .5       1.2       1.8       2.5
       2.0       1.8       1.2        .9
CRED              0.      -11.      250.
CO               1.2        0.        .5      -50.        0.        .5
      12.9      19.4      14.2      11.6      11.6      11.6      11.6
      12.9      14.2      15.5      20.7
CALC              .8       .08        0.        0.        0.
```

TABLE 12. EXAMPLE INPUTS FOR USING THE EKMA OPTION

```
TITL
EXAMPLE OF EKMA OPTION
PLAC          38.629    90.206        6.     1988.        6.       21.
TEST CITY
DILU            250.     1700.        0.        0.        0.
TEMP             11.      294.      296.      299.      301.      304.
          305.  307.      308.      306.      305.      304.      302.
WATE             11.     29.95
           80.   75.       50.       45.       40.       35.       30.
           30.   30.       30.       35.       40.
TRAN              0.       .04        0.       .03        0.      .002
MASS            -11.       .64       .08      250.
          9.42  7.68      7.54      5.21      3.23      2.24      2.18
          1.75  1.72      2.10      1.12
          8.11  6.18      5.65      4.11      2.76      1.90      1.91
          1.60  1.42      1.78       .90
BIOG            -11.        2.      250.
ISOP              0.     .0001        0.        0.     .0001        0.
      68.12
            0.    0.        .1        .3        .8       1.0       1.5
           1.3   1.0        .8        .6
APIN              1.     .0001        0.        0.     .0001        0.
     136.24
            0.    .5       1.5        0.        0.        0.        6.
            0.
            0.    0.        .2        .5       1.2       1.8       2.5
           2.0   1.8       1.2        .9
CRED              0.      -11.      250.
CO               1.2        0.        .5      -50.        0.        .5
          12.9  19.4      14.2      11.6      11.6      11.6      11.6
          12.9  14:2      15.5      20.7
EKMA             .15        8.      -10.        1.        0.        0.
            0.   .04        0.      .024        0.      .002
           .64   .08        0.        0.        0.
```

existing, or base case, conditions. This can be accomplished by using the same input stream that was used in the previous example, but simply replacing the EKMA option with the ISOP option (see Table 13). Since no other information is included on the ISOP input record, default values are used to determine the NMOC and NO_x scales on the resultant diagram. Appendix F contains the OZIPM-4 generated output.

6.5 GENERATION OF FUTURE CASE DIAGRAM WITH THE ISOP OPTION

The final OZIPM-4 application example is another follow-on to the preceding two examples. The isopleth diagram described in the preceding section represented base case conditions. Assume now that a future case diagram is desired in order to reflect projected changes in manmade transport and future CO emissions. In this example, manmade transport of organic compounds from 0.030 ppmC to 0.024 ppmC.[—] CO emissions and the initial CO concentration have been reduced by 50 percent. This is done by revising the individual values in the CREDIT option. The future change field within the CREDITIT option is used only with the EKMA option. As shown in Table 14, these are the only inputs that are changed from those needed to generate the base case diagrams. Appendix G contains the output, which differs only slightly from that in Appendix F. The base and future case diagrams shown in these appendices could then be used to compute the VOC emission reduction that is needed to lower the ozone peak observed on this day to a level of 0.12 ppm.

[—] Such an estimate is arrived at by using Figure 3 of this document.

TABLE 13. EXAMPLE INPUTS FOR GENERATING A BASE CASE ISOPLETH DIAGRAM

```
TITL
EXAMPLE OF BASE CASE ISOPLETH
PLAC          38.629    90.206        6.     1988.        6.       21.
TEST CITY
DILU            250.     1700.        0.        0.        0.
TEMP             11.      294.      296.      299.      301.      304.
      305.      307.      308.      306.      305.      304.      302.
WATE             11.     29.95
       80.       75.       50.       45.       40.       35.       30.
       30.       30.       30.       35.       40.
TRAN              0.       .04        0.       .03        0.      .002
MASS            -11.       .64       .08      250.
      9.42      7.68      7.54      5.21      3.23      2.24      2.18
      1.75      1.72      2.10      1.12
      8.11      6.18      5.65      4.11      2.76      1.90      1.91
      1.60      1.42      1.78       .90
BIOG            -11.        2.      250.
ISOP              0.     .0001        0.        0.     .0001        0.
     68.12
        0.        0.        .1        .3        .8       1.0       1.5
       1.3       1.0        .8        .6
APIN              1.     .0001        0.        0.     .0001        0.
    136.24
        0.        .5       1.5        0.        0.        0.        6.
        0.
        0.        0.        .2        .5       1.2       1.8       2.5
       2.0       1.8       1.2        .9
CRED              0.      -11.      250.
CO               1.2        0.        .5      -50.        0.        .5
      12.9      19.4      14.2      11.6      11.6      11.6      11.6
      12.9      14.2      15.5      20.7
PLOT              0.        0.        0.        0.        0.        0.
ISOP             2.0       .28        1.        0.        1.
       .15
```

TABLE 14. EXAMPLE INPUTS FOR GENERATING A FUTURE CASE ISOPLETH DIAGRAM

```
TITL
EXAMPLE OF FUTURE CASE ISOPLETH
PLAC              38.629    90.206        6.     1988.        6.       21.
TEST CITY
DILU                250.     1700.        0.        0.        0.
TEMP                 11.      294.      296.      299.      301.      304.
          305.      307.      308.      306.      305.      304.      302.
WATE                 11.     29.95
           80.       75.       50.       45.       40.       35.       30.
           30.       30.       30.       35.       40.
TRAN                  0.       .04        0.      .024        0.      .002
MASS                -11.       .64       .08      250.
          9.42      7.68      7.54      5.21      3.23      2.24      2.18
          1.75      1.72      2.10      1.12
          8.11      6.18      5.65      4.11      2.76      1.90      1.91
          1.60      1.42      1.78       .90
BIOG                -11.        2.      250.
ISOP                  0.     .0001        0.        0.     .0001        0.
         68.12
            0.        0.        .1        .3        .8       1.0       1.5
           1.3       1.0        .8        .6
APIN                  1.     .0001        0.        0.     .0001        0.
        136.24
            0.        .5       1.5        0.        0.        0.        6.
            0.
            0.        0.        .2        .5       1.2       1.8       2.5
           2.0       1.8       1.2        .9
CRED                  0.      -11.      250.
CO                  -1.2        0.        .5      -50.        0.        .5
          6.45       9.7       7.1       5.8       5.8       5.8       5.8
          6.45      7.12      7.75     10.35
PLOT                  0.        0.        0.        0.        0.        0.
ISOP                 2.0       .28        1.        0.        1.
           .12
```

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APPENDIX A

CARBON BOND 4 MECHANISM

```
THE REACTIONS                                                            RATE CONSTANT  ACT. ENERGY(K)

  1    NO2                      =      NO    +    O                       1.000E+00     0.000E+00

  2    O                        =      O3                                 4.323E+06    -1.175E+03

  3    O3   +    NO             =      NO2                                2.664E+01     1.370E+03

  4    O    +    NO2            =      NO                                 1.375E+04     0.000E+00

  5    O    +    NO2            =      NO3                                2.309E+03    -6.870E+02

  6    O    +    NO             =      NO2                                2.438E+03    -6.020E+02

  7    NO2  +    O3             =      NO3                                4.731E-02     2.450E+03

  8    O3                       =      O                                  5.300E-02     0.000E+00

  9    O3                       =      O1D                                1.000E+00     0.000E+00

 10    O1D                      =      O                                  4.246E+05    -3.900E+02

 11    O1D  +    H2O            =    2 OH                                 3.260E+00     0.000E+00

 12    O3   +    OH             =      HO2                                1.000E+02     9.400E+02

 13    O3   +    HO2            =      OH                                 3.000E+00     5.800E+02

 14    NO3                      = 0.89 NO2   + 0.89 O     + 0.11 NO       3.390E+01     0.000E+00

 15    NO3  +    NO             =    2 NO2                                4.416E+04    -2.500E+02

 16    NO3  +    NO2            =      NO    +    NO2                     5.901E-01     1.230E+03

 17    NO3  +    NO2            =      N2O5                               1.853E+03    -2.560E+02

 18    N2O5 +    H2O            =    2 HNO3                               1.900E-06     0.000E+00

 19    N2O5                     =      NO3   +    NO2                     2.776E+00     1.090E+04

 20    NO   +    NO             =    2 NO2                                1.539E-04    -5.300E+02

 21    NO   +    NO2  +    H2O  =    2 HNO2                               1.600E-11     0.000E+00

 22    NO   +    OH             =      HNO2                               9.799E+03    -8.060E+02

 23    HNO2                     =      NO    +    OH                      1.975E-01     0.000E+00

 24    OH   +    HNO2           =      NO2                                9.770E+03     0.000E+00

 25    HNO2 +    HNO2           =      NO    +    NO2                     1.500E-05     0.000E+00
```

THE REACTIONS														RATE CONSTANT	ACT. ENERGY(K)
26	NO2	+	OH			=	HNO3							1.682E+04	-7.130E+02
27	OH	+	HNO3			=	NO3							2.179E+02	-1.000E+03
28	HO2	+	NO			=	OH	+	NO2					1.227E+04	-2.400E+02
29	HO2	+	NO2			=	PNA							2.025E+03	-7.490E+02
30	PNA					=	HO2	+	NO2					5.115E-00	1.012E+04
31	OH	+	PNA			=	NO2							6.833E+03	-3.800E+02
32	HO2	+	HO2			=	H2O2							4.144E+03	-1.150E+03
33	HO2	+	HO2	+	H2O	=	H2O2							2.181E-01	-5.800E+03
34	H2O2					=	2 OH							1.890E-01	0.000E+00
35	OH	+	H2O2			=	HO2							2.520E+03	1.870E+02
36	OH	+	CO			=	HO2							3.220E+02	0.000E+00
37	FORM	+	OH			=	HO2	+	CO					1.500E+04	0.000E+00
38	FORM					=	2 HO2	+	CO					1.000E+00	0.000E+00
39	FORM					=	CO							1.000E+00	0.000E+00
40	FORM	+	O			=	OH	+	HO2	+	CO			2.370E+02	1.550E+03
41	FORM	+	NO3			=	HNO3	+	HO2	+	CO			9.300E-01	0.000E+00
42	ALD2	+	O			=	C2O3	+	OH					6.360E+02	9.860E+02
43	ALD2	+	OH			=	C2O3							2.400E+04	-2.500E+02
44	ALD2	+	NO3			=	C2O3	+	HNO3					3.700E+00	0.000E+00
45	ALD2					=	FORM	+	2 HO2	+	CO	+	XO2	1.000E+00	0.000E+00
46	C2O3	+	NO			=	FORM	+	NO2	+	HO2	+	XO2	1.832E+04	-2.500E+02
47	C2O3	+	NO2			=	PAN							1.223E+04	-5.500E+03
48	PAN					=	C2O3	+	NO2					2.220E-02	1.400E+04
49	C2O3	+	C2O3			=	2 FORM	+	2 XO2	+	2 HO2			3.700E+03	0.000E+00
50	C2O3	+	HO2			=	0.79 FORM	+	0.79 XO2	+	0.79 HO2	+	0.79 OH	9.600E+03	0.000E+00

```
THE REACTIONS                                                      RATE CONSTANT  ACT. ENERGY(K)

51      OH                    =       FORM +      XO2  +      HO2               2.100E+01     1.710E+03

52      PAR  +      OH        =  0.87 XO2   + 0.13 XO2N  + 0.11 HO2   + 0.11 ALD2   1.203E+03     0.000E+00
                               - 0.11 PAR   + 0.76 ROR

53      ROR                   =  0.96 XO2   +  1.1 ALD2  + 0.94 HO2   -  2.1 PAR    1.371E+05     8.000E+03
                               + 0.04 XO2N  + 0.02 ROR

54      ROR                   =       HO2                                       9.545E+04     0.000E+00

55      ROR  +      NO2       =                                                 2.200E+04     0.000E+00

56      O    +      OLE       =  0.63 ALD2  + 0.38 HO2   + 0.28 XO2   +  0.3 CO     5.920E+03     3.240E+02
                               +  0.2 FORM  + 0.02 XO2N  + 0.22 PAR   +  0.2 OH

57      OH   +      OLE       =       FORM  +      ALD2  -      PAR   +      XO2    4.200E+04    -5.040E+02
                               +    - HO2

58      O3   +      OLE       =   0.5 ALD2  + 0.74 FORM  + 0.22 XO2   +  0.1 OH     1.800E-02     2.105E+03
                               + 0.33 CO    + 0.44 HO2   -      PAR

59      NO3  +      OLE       =  0.91 XO2   +      FORM  + 0.09 XO2N  +      ALD2   1.135E+01     0.000E+00
                               +      NO2   -      PAR

60      O    +      ETH       =       FORM  +  1.7 HO2   +      CO    +  0.7 XO2    1.080E+03     7.920E+02
                               +  0.3 OH

61      OH   +      ETH       =       XO2   + 1.56 FORM  + 0.22 ALD2  +      HO2    1.192E+04    -4.110E+02

62      O3   +      ETH       =       FORM  + 0.42 CO    + 0.12 HO2                 2.702E-03     2.633E+03

63      TOL  +      OH        =  0.44 HO2   + 0.08 XO2   + 0.36 CRES  + 0.56 TO2    9.150E+03    -3.220E+02

64      TO2  +      NO        =   0.9 NO2   +  0.9 HO2   +  0.9 OPEN                1.200E+04     0.000E+00

65      TO2                   =       CRES  +      HO2                              2.500E+02     0.000E+00

66      OH   +      CRES      =   0.4 CRO   +  0.6 XO2   +  0.6 HO2   +  0.3 OPEN   6.100E+04     0.000E+00

67      CRES +      NO3       =       CRO   +      HNO3                             3.250E+04     0.000E+00

68      CRO  +      NO2       =                                                 2.000E+04     0.000E+00

69      OPEN                  =       C2O3  +      HO2   +      CO                  8.400E+00     0.000E+00

70      OPEN +      OH        =       XO2   +    2 CO    +    2 HO2   +      C2O3   4.400E+04     0.000E+00
                               +      FORM
```

```
THE REACTIONS                                                          RATE CONSTANT  ACT. ENERGY(K)

 71     OPEN  +    O3             =  0.03 ALD2  + 0.62 C2O3  +  0.7 FORM  + 0.03 XO2     1.500E-02     5.000E+02
                                   + 0.69 CO    + 0.08 OH    + 0.76 HO2   +  0.2 MGLY

 72     OH    +    XYL            =   0.7 HO2   +  0.3 XO2   +  0.2 CRES  +  0.8 MGLY    3.620E+04    -1.160E+02
                                   +  1.1 PAR   +  0.3 TO2

 73     OH    +    MGLY           =       XO2   +      C2O3                              2.600E+04     0.000E+00

 74     MGLY                      =       C2O3  +      HO2   +      CO                   8.960E+00     0.000E+00

 75     O     +    ISOP           =   0.6 HO2   +  0.8 ALD2  + 0.55 OLE   +  0.3 XO2     2.700E+04     0.000E+00
                                   +  0.5 CO    + 0.45 ETH   +  0.9 PAR

 76     OH    +    ISOP           =       XO2   +      FORM  + 0.67 HO2   + 0.13 XO2N    1.420E+05     0.000E+00
                                   +      ETH   +  0.4 MGLY  +  0.2 C2O3  +  0.2 ALD2

 77     O3    +    ISOP           =       FORM  +  0.4 ALD2  + 0.55 ETH   +  0.2 MGLY    1.800E-02     0.000E+00
                                   +  0.1 PAR   + 0.06 CO    + 0.44 HO2   +  0.1 OH

 78     NO3   +    ISOP           =       XO2N                                           4.700E+02     0.000E+00

 79     XO2   +    NO             =       NO2                                            1.200E+04     0.000E+00

 80     XO2N  +    NO             =                                                      1.000E+03     0.000E+00

 81     XO2   +    XO2            =                                                      2.000E+03    -1.300E+03

 82     NR                        =       NR                                             1.000E+00     0.000E+00
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THE FOLLOWING PHOTOLYSIS RATE CONSTANTS ARE USED

REACTION NO.	SPECIES *	ZENITH ANGLE (DEG) 0	10	20	30	40	50	60	70	78	86
1	NO2	5.89E-01	5.85E-01	5.71E-01	5.47E-01	5.09E-01	4.54E-01	3.74E-01	2.58E-01	1.34E-01	2.42E-02
8	O3	3.12E-02	3.10E-02	3.03E-02	2.90E-02	2.70E-02	2.40E-02	1.98E-02	1.37E-02	7.11E-03	1.28E-03
9	O3	2.72E-03	2.62E-03	2.36E-03	1.96E-03	1.46E-03	9.44E-04	4.62E-04	1.39E-04	2.95E-05	3.15E-06
14	NO3	2.00E+01	1.98E+01	1.94E+01	1.85E+01	1.73E+01	1.54E+01	1.27E+01	8.74E+00	4.55E+00	3.20E-01
23.	HNO2	1.16E-01	1.16E-01	1.13E-01	1.08E-01	1.01E-01	8.96E-02	7.39E-02	5.09E-02	2.65E-02	4.78E-03
34	H2O2	6.40E-04	6.34E-04	6.12E-04	5.73E-04	5.15E-04	4.36E-04	3.27E-04	1.95E-04	8.79E-05	2.40E-05
38	FORM	2.18E-03	2.14E-03	2.03E-03	1.86E-03	1.60E-03	1.27E-03	8.73E-04	4.48E-04	1.72E-04	4.28E-05
39	FORM	3.39E-03	3.35E-03	3.24E-03	3.03E-03	2.72E-03	2.30E-03	1.73E-03	1.03E-03	4.65E-04	1.27E-04
45	ALD2	3.47E-04	3.38E-04	3.14E-04	2.75E-04	2.22E-04	1.61E-04	9.61E-05	4.07E-05	1.22E-05	2.27E-06
69	OPEN	1.83E-02	1.80E-02	1.71E-02	1.56E-02	1.34E-02	1.07E-02	7.33E-03	3.76E-03	1.44E-03	3.60E-04
74	MGLY	1.95E-02	1.92E-02	1.82E-02	1.67E-02	1.43E-02	1.14E-02	7.82E-03	4.01E-03	1.54E-03	3.84E-04

APPENDIX B

CBM-4 CARBON BOND GROUPS FOR ORGANIC SPECIES

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES (IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
1,1,1-TRICHLOROETHANE	133.40	2.0
1,1,2-TRICHLOROETHANE	133.40	2.0
1,2,3,4-TETRAMETHYLBENZENE	134.22	10.0
1,2,3,5-TETRAMETHYLBENZENE	134.22	10.0
1,2,3-TRIMETHYLBENZENE	120.19	9.0
1,2,4,5-TETRAMETHYLBENZENE	134.22	10.0
1,2,4-TRIMETHYLBENZENE	120.19	9.0
1,2-DIETHYLBENZENE	134.22	10.0
1,2-DIMETHYL-3-ETHYLBENZENE	134.22	10.0
1,2-DIMETHYL-4-ETHYLBENZENE	134.22	10.0
1,3,5-TRIMETHYLBENZENE	120.19	9.0
1,3-BUTADIENE	54.09	4.0
1,3-DIETHYLBENZENE	134.22	10.0
1,4-BUTANEDIOL	90.12	4.0
1,4-DIETHYLBENZENE	134.22	10.0
1-BUTENE	56.11	4.0
1-BUTYNE	54.09	4.0
1-CHLOROBUTANE	92.57	4.0
1-DECENE	140.27	10.0
1-ETHOXY-2-PROPANOL	104.15	5.0
1-HEPTENE	98.19	7.0
1-HEXENE	84.16	6.0
1-METHYLCYCLOHEXENE	96.17	7.0
1-METHYL-2-ETHYLBENZENE	120.19	9.0
1-METHYL-3-ETHYLBENZENE	120.19	9.0
1-METHYL-3-ISOPROPYLBENZENE	134.22	10.0
1-METHYL-3-N-PROPYLBENZENE	134.22	10.0
1-METHYL-4-ISOPROPYLBENZENE	134.22	10.0
1-NONENE	126.24	9.0
1-OCTENE	112.21	8.0
1-PENTENE	70.13	5.0
1-UNDECENE	154.29	11.0
2,2,3-TRIMETHYLBUTANE	100.20	7.0
2,2,3-TRIMETHYLPENTANE	114.23	8.0
2,2,4-TRIMETHYLPENTANE	114.23	8.0
2,2,5-TRIMETHYLHEXANE	128.26	9.0
2,2-DICHLORONITROANILINE	207.02	6.0
2,2-DIMETHYLBUTANE	86.18	6.0
2,2-DIMETHYLHEXANE	114.23	8.0
2,2-DIMETHYLPROPANE	72.15	5.0
2,3,3-TRIMETHYLPENTANE	114.23	8.0
2,3,3-TRIMETHYL-1-BUTENE	98.19	7.0
2,3,4-TRIMETHYLPENTANE	114.23	8.0
2,3,5-TRIMETHYLHEXANE	128.26	9.0
2,3-DIMETHYLBUTANE	86.18	6.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES (IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
2,3-DIMETHYLHEPTANE	128.26	9.0
2,3-DIMETHYLHEXANE	114.23	8.0
2,3-DIMETHYLOCTANE	142.28	10.0
2,3-DIMETHYLPENTANE	100.20	7.0
2,3-DIMETHYL-1-BUTENE	84.16	6.0
2,4,4-TRIMETHYL-1-PENTENE	112.21	8.0
2,4,5-TRIMETHYLHEPTANE	142.29	10.0
2,4-DIMETHYLHEPTANE	128.26	9.0
2,4-DIMETHYLHEXANE	114.23	8.0
2,4-DIMETHYLOCTANE	142.28	10.0
2,4-DIMETHYLPENTANE	100.20	7.0
2,5-DIMETHYLHEPTANE	128.26	9.0
2,5-DIMETHYLHEXANE	114.23	8.0
2,6-DIMETHYLOCTANE	142.28	10.0
2,6-DIMETHYLSTYRENE	132.20	10.0
2-BUTYLTETRAHYDROFURAN	128.21	8.0
2-BUTYNE	54.09	4.0
2-ETHYLHEXANOL	130.23	8.0
2-ETHYL-1-BUTENE	84.16	6.0
2-ETHYL-1-HEXANOL	130.23	8.0
2-FURFURAL	96.08	5.0
2-HEXENE	84.16	6.0
2-METHYLDECANE	156.31	11.0
2-METHYLHEPTANE	114.23	8.0
2-METHYLHEXANE	100.20	7.0
2-METHYLOCTANE	128.26	9.0
2-METHYLPENTANE	86.18	6.0
2-METHYLPROPANE	58.12	4.0
2-METHYLPROPENE	56.11	4.0
2-METHYLPROPENE	56.11	4.0
2-METHYL-1,3-BUTADIENE	68.12	5.0
2-METHYL-1-BUTENE	70.13	5.0
2-METHYL-1-PENTENE	84.16	6.0
2-METHYL-2-BUTENE	70.13	5.0
2-METHYL-2-PENTENE	84.16	6.0
2-METHYL-3-HEXANONE	114.19	7.0
2-(2-BUTOXYETHOXY)-ETHANOL	162.26	8.0
3,3-DIMETHYLPENTANE	100.20	7.0
3,4-DIMETHYLOCTANE	142.28	10.0
3,5,5-TRIMETHYLHEXANE	128.26	9.0
3,5-DIMETHYLHEPTANE	128.26	9.0
3-HEPTENE	98.19	7.0
3-METHYLHEPTANE	114.23	8.0
3-METHYLHEXANE	100.20	7.0
3-METHYLOCTANE	128.26	9.0
3-METHYLPENTANE	86.18	6.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES (IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
3-METHYL-1-BUTENE	70.13	5.0
3-METHYL-1-PENTENE	84.16	6.0
3-METHYL-CIS-2-PENTENE	84.16	6.0
3-METHYL-TRANS-2-PENTENE	84.16	6.0
3-(CHLOROMETHYL)-HEPTANE	148.68	8.0
4,4-METHYLENE DIANILINE	198.27	13.0
4-METHYLANILINE	107.15	7.0
4-METHYLHEPTANE	114.23	8.0
4-METHYLNONANE	142.28	10.0
4-METHYLOCTANE	128.26	9.0
4-METHYL-1-PENTENE	84.16	6.0
4-METHYL-CIS-2-PENTENE	84.16	6.0
4-METHYL-TRANS-2-PENTENE	84.16	6.0
4-PHENYL-1-BUTENE	132.20	10.0
ACENAPHTHENE	154.21	12.0
ACENAPHTHYLENE	152.20	12.0
ACETALDEHYDE	44.05	2.0
ACETIC ACID	60.05	2.0
ACETIC ANHYDRIDE	102.09	4.0
ACETONE	58.08	3.0
ACETYLENE	26.04	2.0
ACROLEIN (PROPENAL)	56.06	3.0
ACRYLIC ACID	72.06	3.0
ACRYLONITRILE	53.06	3.0
ADIPIC ACID	146.14	6.0
ALIPHATICS (per carbon)	14.03	1.0
ALKENE KETONE	72.11	4.0
AMINOANTHRAQUINONE	223.23	14.0
ANILINE	93.13	6.0
ANTHANTHRENE	302.37	24.0
ANTHRACENE	178.23	14.0
ANTHRAQUINONE	208.22	14.0
A-PINENE	136.24	10.0
BENZALDEHYDE	106.12	7.0
BENZENE	78.11	6.0
BENZOIC ACID	122.12	7.0
BENZOPYRENES	252.31	20.0
BENZOTHIAZOLE	135.18	7.0
BENZO(a)ANTHRACENE	228.29	18.0
BENZO(a)PYRENE	252.31	20.0
BENZO(b)FLUORANTHENE	252.31	20.0
BENZO(c)PHENANTHRENE	228.29	18.0
BENZO(e)PYRENE	252.31	20.0
BENZO(g,h,i)FLUORANTHENE	226.28	18.0
BENZO(g,h,i)PERYLENE	276.34	22.0
BENZO(k)FLUORANTHENE	252.31	20.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES
(IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
BENZYLCHLORIDE	126.59	7.0
BIPHENYL	154.21	12.0
BIPHENYLOL	170.22	12.0
BROMODINITROANILINE	262.02	6.0
BROMODINITROBENZENE	247.00	6.0
BUTENE	56.11	4.0
BUTOXYBUTENE	128.21	8.0
BUTOXYETHOXYETHANOL	162.23	8.0
BUTOXYETHOXYETHANOL ACETATE	220.26	10.0
BUTYL CARBITOL	162.23	8.0
BUTYL CELLOSOLVE	118.20	6.0
BUTYLACRYLATE	128.17	7.0
BUTYLBENZENE	134.22	10.0
BUTYLBENZOATE	178.23	11.0
BUTYLBENZYLPHTHALATE	312.36	19.0
BUTYLCYCLOHEXANE	140.27	10.0
BUTYLISOPROPYLPHTHALATE	264.32	15.0
BUTYRALDEHYDE	72.11	4.0
B-PHELLANDRENE	136.24	10.0
B-PINENE	136.24	10.0
C1 COMPOUNDS (DIESEL EXHAUST)	16.04	1.0
C10 AROMATIC	134.22	10.0
C10 COMPOUNDS (DIESEL EXHAUST)	140.00	10.0
C10 OLEFINS	140.27	10.0
C10 PARAFFINS	142.28	10.0
C10H12	132.20	10.0
C10H16	136.24	10.0
C10H160	152.24	10.0
C11 COMPOUNDS (DIESEL EXHAUST)	154.00	11.0
C11 OLEFINS	154.29	11.0
C11 PARAFFIN	156.31	11.0
C11H10	142.20	11.0
C11H140	162.23	11.0
C12 COMPOUNDS (DIESEL EXHAUST)	168.00	12.0
C12 OLEFINS	168.32	12.0
C12 PARAFFIN	170.34	12.0
C12H22	166.31	12.0
C13 COMPOUNDS (DIESEL EXHAUST)	182.00	13.0
C13 PARAFFIN	184.36	13.0
C14 COMPOUNDS (DIESEL EXHAUST)	196.00	14.0
C15 COMPOUNDS (DIESEL EXHAUST)	210.00	15.0
C16 BRANCHED ALKANE	226.44	16.0
C16 COMPOUNDS (DIESEL EXHAUST)	224.00	16.0
C17 COMPOUNDS (DIESEL EXHAUST)	238.00	17.0
C18 COMPOUNDS (DIESEL EXHAUST)	252.00	18.0
C19 COMPOUNDS (DIESEL EXHAUST)	266.00	19.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES (IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
C2 ALKYLANTHRACENES	206.29	16.0
C2 ALKYLBENZANTHRACENE	256.35	20.0
C2 ALKYLBENZOPHENANTHRENE	256.35	20.0
C2 ALKYLCHRYSENES	256.35	20.0
C2 ALKYLCYCLOHEXANE	112.21	8.0
C2 ALKYLINDAN	146.23	11.0
C2 ALKYLNAPTHALENE	156.23	12.0
C2 ALKYLPHENANTHRENES	206.29	16.0
C2 COMPOUNDS (DIESEL EXHAUST)	28.55	2.0
C20 COMPOUNDS (DIESEL EXHAUST)	280.00	20.0
C21 COMPOUNDS (DIESEL EXHAUST)	294.00	21.0
C22 COMPOUNDS (DIESEL EXHAUST)	308.00	22.0
C23 COMPOUNDS (DIESEL EXHAUST)	322.00	23.0
C24 COMPOUNDS (DIESEL EXHAUST)	336.00	24.0
C25 COMPOUNDS (DIESEL EXHAUST)	350.00	25.0
C26 COMPOUNDS (DIESEL EXHAUST)	364.00	26.0
C27 COMPOUNDS (DIESEL EXHAUST)	378.00	27.0
C28 COMPOUNDS (DIESEL EXHAUST)	392.00	28.0
C29 COMPOUNDS (DIESEL EXHAUST)	406.00	29.0
C3 ALKYLCYCLOHEXANE	126.24	9.0
C3 ALKYLSTYRENE	146.23	11.0
C3 COMPOUNDS (DIESEL EXHAUST)	42.08	3.0
C3 PARAFFIN	44.10	3.0
C30 COMPOUNDS (DIESEL EXHAUST)	420.00	30.0
C31 COMPOUNDS (DIESEL EXHAUST)	434.00	31.0
C32 COMPOUNDS (DIESEL EXHAUST)	448.00	32.0
C33 COMPOUNDS (DIESEL EXHAUST)	462.00	33.0
C34 COMPOUNDS (DIESEL EXHAUST)	476.00	34.0
C35 COMPOUNDS (DIESEL EXHAUST)	490.00	35.0
C36 COMPOUNDS (DIESEL EXHAUST)	504.00	36.0
C37 COMPOUNDS (DIESEL EXHAUST)	518.00	37.0
C38 COMPOUNDS (DIESEL EXHAUST)	532.00	38.0
C39 COMPOUNDS (DIESEL EXHAUST)	546.00	39.0
C3/C4/C5 ALKYLBENZENES	134.22	10.0
C4 ALKYLPHENOLS	150.22	10.0
C4 ALKYLSTYRENES	160.26	12.0
C4 COMPOUNDS (DIESEL EXHAUST)	57.08	4.0
C4 OLEFIN	56.11	4.0
C4 PARAFFIN	58.12	4.0
C4 SUBSTITUTED CYCLOHEXANE	140.27	10.0
C4 SUBSTITUTED CYCLOHEXANONE	154.25	10.0
C40 COMPOUNDS (DIESEL EXHAUST)	560.00	40.0
C41 COMPOUNDS (DIESEL EXHAUST)	574.00	41.0
C42 COMPOUNDS (DIESEL EXHAUST)	588.00	42.0
C43 COMPOUNDS (DIESEL EXHAUST)	602.00	43.0
C5 ALKYL CYCLOHEXANE	154.29	11.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES
(IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
C5 ALKYLBENZENES	148.25	11.0
C5 ALKYLBENZENES (UNSATURATED)	146.23	11.0
C5 ALKYLPHENOLS	164.25	11.0
C5 COMPOUNDS (DIESEL EXHAUST)	71.00	5.0
C5 ESTER	130.19	7.0
C5 OLEFIN	70.13	5.0
C5 PARAFFIN	72.15	5.0
C5 PARAFFIN/OLEFIN	70.13	5.0
C5 SUBSTITUTED CYCLOHEXANE	154.29	11.0
C5H100	86.13	5.0
C6 ALKYLBENZENE	162.27	12.0
C6 COMPOUNDS (DIESEL EXHAUST)	79.12	6.0
C6 OLEFINS	84.16	6.0
C6 PARAFFIN	86.18	6.0
C6 SUBSTITUTED CYCLOHEXANE	168.32	12.0
C6H1803SI3	222.46	6.0
C7 ALKYLBENZENE	176.30	13.0
C7 COMPOUNDS (DIESEL EXHAUST)	93.18	7.0
C7 CYCLOPARAFFINS	98.19	7.0
C7 OLEFINS	98.19	7.0
C7 PARAFFINS	100.20	7.0
C7H12	96.17	7.0
C7H120	112.17	7.0
C7-C16	156.31	11.0
C8 COMPOUNDS (DIESEL EXHAUST)	112.00	8.0
C8 CYCLOPARAFFINS	112.21	8.0
C8 OLEFINS	112.21	8.0
C8 PARAFFIN	114.23	8.0
C8 PHENOLS	122.17	8.0
C8H14	110.20	8.0
C8H2404SI4	296.62	8.0
C9 COMPOUNDS (DIESEL EXHAUST)	126.00	9.0
C9 CYCLOPARAFFINS	126.24	9.0
C9 OLEFINS	126.24	9.0
C9 PARAFFIN	128.26	9.0
C9 PHENOLS	136.19	9.0
CAMPHENE	136.24	10.0
CAPROLACTAM	113.16	6.0
CARBITOL	134.17	6.0
CARBON DISULFIDE	76.14	1.0
CARBON TETRACHLORIDE	153.82	1.0
CARBONYL SULFIDE	60.07	1.0
CARYOPHYLLENE	204.36	15.0
CELLOSOLVE	90.14	4.0
CELLOSOLVE ACETATE	132.16	6.0
CHLOROBENZENE	112.56	6.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES
(IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
CHLORODIFLUOROMETHANE	86.47	1.0
CHLOROFORM	119.38	1.0
CHLOROPENTAFLUOROETHANE	154.47	2.0
CHLOROPRENE	88.54	4.0
CHLOROTRIFLUOROMETHANE	104.46	1.0
CHRYSENE	228.29	18.0
CIS-1,4-DIMETHYLCYCLOHEXANE	112.21	8.0
CIS-2-BUTENE	56.11	4.0
CIS-2-HEPTENE	98.19	7.0
CIS-2-HEXENE	84.16	6.0
CIS-2-OCTENE	112.21	8.0
CIS-2-PENTENE	70.13	5.0
CIS-3-HEXENE	84.16	6.0
CORONENE	300.36	24.0
CREOSOTE	130.19	11.0
CRESOL	108.14	7.0
CROTONALDEHYDE	70.09	4.0
CUMENE (ISOPROPYL BENZENE)	120.19	9.0
CYCLOHEPTANE	98.19	7.0
CYCLOHEXANE	84.16	6.0
CYCLOHEXANOL	100.16	6.0
CYCLOHEXANONE	98.14	6.0
CYCLOHEXENE	82.14	6.0
CYCLOPENTAANTHRACENES	204.27	16.0
CYCLOPENTANE	70.13	5.0
CYCLOPENTAPHENANTHRENES	204.27	16.0
CYCLOPENTA(c,d)PYRENE	228.29	18.0
CYCLOPENTENE	68.12	5.0
CYCLOPENTYLCYCLOPENTANE	138.25	10.0
DECALINS	138.25	10.0
DENATURANT	32.04	1.0
DIACETONE ALCOHOL	116.18	6.0
DIBENZANTHRACENES	278.35	22.0
DIBENZOPYRENES	302.37	24.0
DIBENZO(a,h)ANTHRACENE	278.35	22.0
DIBENZPHENANTHRENES	278.35	22.0
DIBUTYL ETHER	130.23	8.0
DIBUTYLPHTHALATE	278.35	16.0
DICHLOROBENZENES	147.00	6.0
DICHLORODIFLUOROMETHANE	120.91	1.0
DICHLOROMETHANE	84.93	1.0
DICHOLROTETRAFLUOROETHANE	170.92	2.0
DIETHYLCYCLOHEXANE	140.27	10.0
DIETHYLENE GLYCOL	106.12	4.0
DIETHYLMETHYLCYCLOHEXANE	154.29	11.0
DIHYDRONAPTHALENE	130.19	10.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES (IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
DIHYDROXYNAPTHALENEDIONE	160.17	10.0
DIISOPROPYLBENZENE	162.27	12.0
DIMETHYL ALKYL AMINES	59.11	3.0
DIMETHYLBENZYLALCOHOL	136.19	9.0
DIMETHYLBUTANE	86.18	6.0
DIMETHYLBUTANEDIOATE	146.14	6.0
DIMETHYLBUTENE	84.16	6.0
DIMETHYLBUTYLCYCLOHEXANE	168.32	12.0
DIMETHYLCYCLOBUTANONE	98.14	6.0
DIMETHYLCYCLOHEXANE	112.21	8.0
DIMETHYLCYCLOPENTANE	98.19	7.0
DIMETHYLCYCLOPENTENES	96.17	7.0
DIMETHYLDECANE	170.34	12.0
DIMETHYLETHER	46.07	2.0
DIMETHYLETHYLBENZOIC ACID	178.23	11.0
DIMETHYLETHYLCYCLOHEXANE	140.27	10.0
DIMETHYLFORMAMIDE	73.09	3.0
DIMETHYLHEPTANES	128.26	9.0
DIMETHYLHEPTANOL	144.26	9.0
DIMETHYLHEXADIENE	110.20	8.0
DIMETHYLHEXANEDIOATE	174.19	8.0
DIMETHYLHEXANES	114.23	8.0
DIMETHYLHEXENE	112.21	8.0
DIMETHYLINDANS	146.23	11.0
DIMETHYLINDENE	144.22	11.0
DIMETHYLNAPHTHYRIDINE	158.20	10.0
DIMETHYLNAPTHALENE	156.23	12.0
DIMETHYLNONANES	156.31	11.0
DIMETHYLOCTANES	142.28	10.0
DIMETHYLOCTANOL	158.32	10.0
DIMETHYLOCTENES	140.27	10.0
DIMETHYLOCTYNE	138.25	10.0
DIMETHYLPENTANE	100.20	7.0
DIMETHYLPENTANEDIOATE	160.17	7.0
DIMETHYLPENTANOL	116.20	7.0
DIMETHYLPENTENE	98.19	7.0
DIMETHYLPHTHALATE	194.19	10.0
DIMETHYLTEREPHTHALATE	194.19	10.0
DIMETHYLUNDECANE	184.36	13.0
DIPHENYLETHANE	182.26	14.0
DIPROPYLENE GLYCOL	134.17	6.0
DIPROPYLPHTHALATE	250.29	14.0
DIVINYLBENZENE	130.19	10.0
DI(ETHYLPHENYL)ETHANE	238.37	18.0
DI-C8 ALKYL PHTHALATE	390.56	24.0
DODECENE	168.32	12.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES (IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
D-LIMONENE	136.24	10.0
EICOSANE.	282.55	20.0
EPICHLOROHYDRIN	92.52	3.0
ETHANE	30.07	2.0
ETHANOLAMINE	61.08	2.0
ETHYL ACETATE	88.11	4.0
ETHYL ACRYLATE	100.12	5.0
ETHYL ALCOHOL	46.07	2.0
ETHYL CHLORIDE	64.51	2.0
ETHYL ETHER	74.12	4.0
ETHYLAMINE	45.08	2.0
ETHYLBENZENE	106.17	8.0
ETHYLBICYCLOHEPTANE	223.42	16.0
ETHYLCYCLOHEXANE	112.21	8.0
ETHYLCYCLOPENTANE	98.19	7.0
ETHYLCYCLOPENTENE	96.17	7.0
ETHYLDIMETHYLBENZENE	134.22	10.0
ETHYLDIMETHYLCYCLOHEXANE	140.27	10.0
ETHYLDIMETHYLOCTANE	170.34	12.0
ETHYLDIMETHYLPENTANE	128.26	9.0
ETHYLDIMETHYLPHENOL	150.22	10.0
ETHYLENE	28.05	2.0
ETHYLENE DIBROMIDE	187.86	2.0
ETHYLENE DICHLORIDE	98.96	2.0
ETHYLENE GLYCOL	62.07	2.0
ETHYLENE OXIDE	44.05	2.0
ETHYLENEAMINES	45.08	2.0
ETHYLFURAN	96.13	6.0
ETHYLHEPTANE	128.26	9.0
ETHYLHEPTENE	126.24	9.0
ETHYLHEXANE	114.23	8.0
ETHYLHEXANOATE	144.21	8.0
ETHYLINDAN	146.23	11.0
ETHYLISOPROPYL ETHER	88.15	5.0
ETHYLMERCAPTAN	62.13	2.0
ETHYLMETHYLCYCLOHEXANE	126.24	9.0
ETHYLMETHYLCYCLOPENTANE	112.21	8.0
ETHYLMETHYLHEXANE	128.26	9.0
ETHYLMETHYLOCTANE	156.31	11.0
ETHYLOCTANE	142.28	10.0
ETHYLOCTENE	140.27	10.0
ETHYLPENTENE	98.19	7.0
ETHYLPHENYLPHENYLETHANE	210.32	16.0
ETHYLPROPYLCYCLOHEXANE	154.29	11.0
ETHYLSTYRENE	132.20	10.0
ETHYLTOLUENE	120.19	9.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES (IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
ETHYL-T-BUTYL ETHER	102.18	6.0
FLUORANTHENE	202.25	16.0
FLUORENE	166.22	13.0
FORMALDEHYDE	30.03	1.0
FORMIC ACID	46.02	1.0
FURFURYL ALCOHOL	98.10	5.0
GLYCEROL	92.09	3.0
GLYCOL	62.07	2.0
GLYCOL ETHER	106.14	4.0
GLYOXAL	58.04	2.0
HENEICOSANE	296.58	21.0
HEPTADIENAL	110.16	7.0
HEPTANE	100.20	7.0
HEPTANONE	114.19	7.0
HEPTENE	98.19	7.0
HEXADECANE	226.44	16.0
HEXADECANOIC ACID	256.43	16.0
HEXADIENAL	96.13	6.0
HEXAFLUOROETHANE	138.01	2.0
HEXAMETHYLENEDIAMINE	116.21	6.0
HEXANAL	100.16	6.0
HEXANE	86.18	6.0
HEXENE	84.16	6.0
HEXYLENE GLYCOL	118.17	6.0
HEXYNE	82.14	6.0
INDANE	118.18	9.0
INDENE	116.16	9.0
INDENO(1,2,3-cd)PYRENE	276.34	22.0
ISOAMYL ALCOHOL	88.15	5.0
ISOAMYLBENZENE	148.25	11.0
ISOBUTANE	58.12	4.0
ISOBUTYL ALCOHOL	74.12	4.0
ISOBUTYLACETATE	116.16	6.0
ISOBUTYLACRYLATE	128.17	7.0
ISOBUTYLBENZENE	134.22	10.0
ISOBUTYLENE	56.11	4.0
ISOBUTYLISOBUTYRATE	144.21	8.0
ISOBUTYRALDEHYDE	72.11	4.0
ISOMERS OF BUTENE	56.11	4.0
ISOMERS OF BUTYLBENZENE	134.22	10.0
ISOMERS OF C10H10	130.19	10.0
ISOMERS OF C10H18	138.25	10.0
ISOMERS OF C11H20	152.28	11.0
ISOMERS OF C9H16	124.23	9.0
ISOMERS OF DECANE	142.28	10.0
ISOMERS OF DIETHYLBENZENE	134.22	10.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES
(IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
ISOMERS OF DODECANE	170.34	12.0
ISOMERS OF ETHYLTOLUENE	120.19	9.0
ISOMERS OF HEPTADECANE	240.47	17.0
ISOMERS OF HEPTANE	100.20	7.0
ISOMERS OF HEXANE	86.18	6.0
ISOMERS OF NONANE	128.26	9.0
ISOMERS OF OCTADECANE	254.50	18.0
ISOMERS OF OCTANE	114.23	8.0
ISOMERS OF PENTADECANE	212.42	15.0
ISOMERS OF PENTANE	72.15	5.0
ISOMERS OF PENTENE	70.13	5.0
ISOMERS OF PROPYLBENZENE	120.19	9.0
ISOMERS OF TETRADECANE	198.39	14.0
ISOMERS OF TRIDECANE	184.36	13.0
ISOMERS OF UNDECANE	156.31	11.0
ISOMERS OF XYLENE	106.17	8.0
ISOOCTANE	114.23	8.0
ISOPENTANE	72.15	5.0
ISOPRENE	68.12	5.0
ISOPROPYL ALCOHOL	60.10	3.0
ISOPROPYLACETATE	102.13	5.0
ISOPROPYLBENZENE	120.19	9.0
ISOPROPYLCYCLOHEXANE	126.24	9.0
ISOPROPYLCYCLOPENTANE	112.21	8.0
ISOPROPYLMETHYLCYCLOHEXANE	140.27	10.0
ISOVALERALDEHYDE	86.13	5.0
LACTOL SPIRITS	114.23	8.0
LIMONENE	136.24	10.0
MALEIC ANHYDRIDE	98.06	4.0
METHANE	16.04	1.0
METHOXYETHOXYBUTANONE	116.16	6.0
METHOXYETHOXYETHANOL	120.15	5.0
METHOXYNAPHTHALENE	158.20	11.0
METHYL ALCOHOL	32.04	1.0
METHYL C11 ESTER	214.35	13.0
METHYL C12 ESTER	228.37	14.0
METHYL C13 ESTER	242.40	15.0
METHYL C14 ESTER	256.43	16.0
METHYL C15 ESTER	270.45	17.0
METHYL C19 ESTER	326.56	21.0
METHYL C20 ESTER	340.59	22.0
METHYLACETATE	74.08	3.0
METHYLACETOPHENONE	134.18	9.0
METHYLACETYLENE (PROPYNE)	40.06	3.0
METHYLACRYLATE	86.09	4.0
METHYLAL	76.11	3.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES (IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
METHYLALLENE	54.09	4.0
METHYLAMYL KETONE	114.19	7.0
METHYLANTHRACENES	192.26	15.0
METHYLBENZANTHRACENES	242.32	19.0
METHYLBENZPHENANTHRENE	242.32	19.0
METHYLBIPHENYL	168.24	13.0
METHYLBUTADIENE	68.12	5.0
METHYLBUTENE	70.13	5.0
METHYLBUTYL KETONE	100.16	6.0
METHYLCARBITOL	120.15	5.0
METHYLCELLOSOLVE	76.11	3.0
METHYLCHLORIDE	50.49	1.0
METHYLCHRYSENES	242.32	19.0
METHYLCYCLOHEXADIENE	94.16	7.0
METHYLCYCLOHEXANE	98.19	7.0
METHYLCYCLOHEXENE	96.17	7.0
METHYLCYCLOOCTANE	126.24	9.0
METHYLCYCLOPENTADIENE	80.13	6.0
METHYLCYCLOPENTANE	84.16	6.0
METHYLCYCLOPENTENE	82.14	6.0
METHYLDECALINS	152.28	11.0
METHYLDECANES	156.31	11.0
METHYLDECENE	154.29	11.0
METHYLDIHYDRONAPHTHALE	144.22	11.0
METHYLDODECANE	184.36	13.0
METHYLDODECANOATE	214.35	13.0
METHYLENE BROMIDE	173.83	1.0
METHYLENE CHLORIDE	84.93	1.0
METHYLENEBIS(C6H4NCO)	250.26	15.0
METHYLENE(b)4-PHENYLISOCYANATE	250.27	15.0
METHYLETHYL KETONE	72.11	4.0
METHYLETHYLHEPTANE	142.28	10.0
METHYLETHYLPENTANOATE	144.21	8.0
METHYLFLUORANTHENES	216.28	17.0
METHYLFORMATE	60.05	2.0
METHYLGLYOXAL	72.06	3.0
METHYLHEPTANE	114.23	8.0
METHYLHEPTANOL	130.26	8.0
METHYLHEPTENE	112.21	8.0
METHYLHEPTYNE	110.20	8.0
METHYLHEXADIENE	96.17	7.0
METHYLHEXANAL	114.19	7.0
METHYLHEXANE	100.20	7.0
METHYLHEXENES	98.19	7.0
METHYLINDANS	132.20	10.0
METHYLINDENE	130.19	10.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES (IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
METHYLISOBUTYL KETONE	100.16	6.0
METHYLISOPROPYLCYCLOHEXANE	140.27	10.0
METHYLMETHACRYLATE	100.12	5.0
METHYLMETHYLPROPENOATE	100.13	5.0
METHYLMYRISTATE	242.40	15.0
METHYLNAPHTHALENES	142.20	11.0
METHYLNONANE	142.28	10.0
METHYLNONENE	140.27	10.0
METHYLOCTANES	128.26	9.0
METHYLPALMITATE	270.45	17.0
METHYLPENTANE	86.18	6.0
METHYLPENTENES	84.16	6.0
METHYLPHENANTHRENES	192.26	15.0
METHYLPROPYLCYCLOHEXANE	140.27	10.0
METHYLPROPYLNONANE	184.36	13.0
METHYLSTEARATE	298.51	19.0
METHYLSTYRENE	118.18	9.0
METHYLUNDECANE	170.34	12.0
METHYL-T-BUTYL ETHER	88.15	5.0
MINERAL SPIRITS	114.00	8.0
MYRCENE	136.24	10.0
M-DICHLOROBENZENE	147.00	6.0
M-DIETHYLBENZENE	134.22	10.0
M-ETHYLTOLUENE	120.19	9.0
M-XYLENE	106.17	8.0
M-XYLENE AND P-XYLENE	106.17	8.0
NAPHTHA	114.00	8.0
NAPTHALENE	128.17	10.0
NITROBENZENE	123.11	6.0
NONADECANE	268.52	19.0
NONADIENE	124.23	9.0
NONANE	128.26	9.0
NONENE	126.24	9.0
NONENONE	140.22	9.0
NONYLPHENOL	220.35	15.0
N-AMYLBENZENE	148.25	11.0
N-BUTANE	58.12	4.0
N-BUTYL ALCOHOL	74.12	4.0
N-BUTYLACETATE	116.16	6.0
N-DECANE	142.28	10.0
N-DODECANE	170.34	12.0
N-HEPTADECANE	240.47	17.0
N-HEXYLBENZENE	162.27	12.0
N-PENTADECANE	212.42	15.0
N-PENTANE	72.15	5.0
N-PENTENE	70.13	5.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES (IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
N-PENTYLCYCLOHEXANE	154.29	11.0
N-PHENYLANILINE	169.23	12.0
N-PROPYL ALCOHOL	60.10	3.0
N-PROPYLACETATE	102.13	5.0
N-PROPYLBENZENE	120.19	9.0
N-TETRADECANE	198.39	14.0
N-TRIDECANE	184.36	13.0
N-UNDECANE	156.31	11.0
OCTAHYDROINDENES	244.00	9.0
OCTAMETHYLCYCLOTETRASILOXANE	296.62	8.0
OCTANE	114.23	8.0
OCTANOL	130.23	8.0
OCTATRIENE	108.18	8.0
OCTENE	112.21	8.0
OXYGENATES	88.11	4.0
O-DICHLOROBENZENE	147.00	6.0
O-ETHYLTOLUENE	120.19	9.0
O-XYLENE	106.17	8.0
PALMITIC ACID	256.43	16.0
PARAFFINS (C16-C34)	352.43	25.0
PARAFFINS (C2-C7)	65.14	4.5
PARAFFINS/OLEFINS (C12-C16)	197.38	14.0
PENTADIENE	68.12	5.0
PENTANOL	88.15	5.0
PENTENYNE	66.10	5.0
PENTYLBENZENE	148.25	11.0
PENTYLCYCLOHEXANE	154.29	11.0
PENTYLIDENECYCLOHEXANE	152.00	11.0
PENTYNE	68.12	5.0
PERCHLOROETHYLENE	165.83	2.0
PERYLENE	252.31	20.0
PHENANTHRENE	178.23	14.0
PHENOL	94.11	6.0
PHENYLISOCYANATE	119.12	7.0
PHENYLNAPHTHALENES	204.27	16.0
PHTHALIC ANHYDRIDE	148.12	8.0
PIPERYLENE	68.12	5.0
POLYETHYLENE GLYCOL	62.07	2.0
PROPADIENE	40.06	3.0
PROPANE	44.10	3.0
PROPENE	42.08	3.0
PROPENYLCYCLOHEXANE	124.23	9.0
PROPIONALDEHYDE	58.08	3.0
PROPIONIC ACID	74.08	3.0
PROPYLBENZENE	120.19	9.0
PROPYLCYCLOHEXANE	126.24	9.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES (IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
PROPYLENE DICHLORIDE	112.99	3.0
PROPYLENE GLYCOL	76.09	3.0
PROPYLENE OXIDE	58.08	3.0
PROPYLHEPTENES	140.27	10.0
PYRENE	202.25	16.0
P-DICHLOROBENZENE	147.00	6.0
P-ETHYLTOLUENE	120.19	9.0
P-TOLUALDEHYDE	120.15	8.0
P-XYLENE	106.17	8.0
SEC-BUTYL ALCOHOL	74.12	4.0
SEC-BUTYLBENZENE	134.22	10.0
SILOXANE	76.08	0.0
STYRENE	104.15	8.0
SUBSTITUTED C9 ESTER (C12)	218.34	13.0
TEREPHTHALIC ACID	166.13	8.0
TERPENES	136.24	10.0
TETRACHLOROBENZENES	215.89	6.0
TETRAFLUOROMETHANE	88.00	1.0
TETRAMETHYLBENZENE	134.22	10.0
TETRAMETHYLCYCLOBUTENE	110.20	8.0
TETRAMETHYLCYCLOPENTANE	126.24	9.0
TETRAMETHYLHEXANE	142.28	10.0
TETRAMETHYLPENTANONE	142.24	9.0
TETRAMETHYLSILANE	88.22	4.0
TETRAMETHYLTHIOUREA	132.22	5.0
TOLUENE	92.14	7.0
TOLUENE DIISOCYANATE	174.16	9.0
TOLUENE ISOCYANATE	133.15	8.0
TOTAL AROMATIC AMINES	93.13	6.0
TOTAL C2-C5 ALDEHYDES	72.12	3.5
TRANS-1-PHENYLBUTENE	132.20	10.0
TRANS-2-BUTENE	56.11	4.0
TRANS-2-HEPTENE	98.19	7.0
TRANS-2-HEXENE	84.16	6.0
TRANS-2-NONENE	126.24	9.0
TRANS-2-PENTENE	70.13	5.0
TRANS-3-HEXENE	84.16	6.0
TRICHLOROBENZENES	181.45	6.0
TRICHLOROFLUOROMETHANE	137.37	1.0
TRICHLOROTRIFLUOROETHANE	187.38	2.0
TRICHOLROETHYLENE	131.39	2.0
TRIETHYLENE GLYCOL	150.17	6.0
TRIFLUOROMETHANE	70.01	1.0
TRIMETHYLAMINE	59.11	3.0
TRIMETHYLBENZENE	120.19	9.0
TRIMETHYLCYCLOHEXANES	126.24	9.0

TABLE B-1

MOLECULAR WEIGHTS & CARBON NUMBERS OF MOLECULES (IN ALPHABETICAL ORDER)

CHEMICAL NAME	MW	CARBON NO
TRIMETHYLCYCLOHEXANOL	142.24	9.0
TRIMETHYLCYCLOPENTANE	112.16	8.0
TRIMETHYLCYCLOPENTANONE	126.20	8.0
TRIMETHYLDECANE	184.36	13.0
TRIMETHYLDECENE	182.35	13.0
TRIMETHYLFLUOROSILANE	92.19	3.0
TRIMETHYLHEPTANES	142.28	10.0
TRIMETHYLHEXANES	128.26	9.0
TRIMETHYLHEXENE	126.24	9.0
TRIMETHYLINDAN	160.26	12.0
TRIMETHYLNONENE	168.32	12.0
TRIMETHYLOCTANES	156.31	11.0
TRIMETHYLPENTADIENE	110.20	8.0
TRIMETHYLPENTANE	114.23	8.0
T-BUTYL ALCOHOL	74.12	4.0
T-BUTYLBENZENE	134.22	10.0
UNIDENTIFIED	86.18	6.0
VINYL ACETATE	86.09	4.0
VINYL CHLORIDE	62.50	2.0
XYLENE BASE ACIDS	230.00	8.0

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1,1,1-TRICHLOROETHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
1,1,2-TRICHLOROETHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
1,2,3,4-TETRAMETHYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1,2,3,5-TETRAMETHYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1,2,3-TRIMETHYLBENZENE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1,2,4,5-TETRAMETHYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1,2,4-TRIMETHYLBENZENE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1,2-DIETHYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1,2-DIMETHYL-3-ETHYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1,2-DIMETHYL-4-ETHYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1,3,5-TRIMETHYLBENZENE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1,3-BUTADIENE	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1,3-DIETHYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1,4-BUTANEDIOL	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1,4-DIETHYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1-BUTENE	1.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-BUTYNE	0.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
1-CHLOROBUTANE	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-DECENE	1.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-ETHOXY-2-PROPANOL	0.00	3.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
1-HEPTENE	1.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-HEXENE	1.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-METHYLCYCLOHEXENE	1.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-METHYL-2-ETHYLBENZENE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1-METHYL-3-ETHYLBENZENE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1-METHYL-3-ISOPROPYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1-METHYL-3-N-PROPYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1-METHYL-4-ISOPROPYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
1-NONENE	1.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-OCTENE	1.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-PENTENE	1.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-UNDECENE	1.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,2,3-TRIMETHYLBUTANE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,2,3-TRIMETHYLPENTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,2,4-TRIMETHYLPENTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,2,5-TRIMETHYLHEXANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,2-DICHLORONITROANILINE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
2,2-DIMETHYLBUTANE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,2-DIMETHYLHEXANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,2-DIMETHYLPROPANE	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,3,3-TRIMETHYLPENTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,3,3-TRIMETHYL-1-BUTENE	0.00	6.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00
2,3,4-TRIMETHYLPENTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,3,5-TRIMETHYLHEXANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,3-DIMETHYLBUTANE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,3-DIMETHYLHEPTANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
2,3-DIMETHYLHEXANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,3-DIMETHYLOCTANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,3-DIMETHYLPENTANE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,3-DIMETHYL-1-BUTENE	0.00	5.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00
2,4,4-TRIMETHYL-1-PENTENE	0.00	7.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00
2,4,5-TRIMETHYLHEPTANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,4-DIMETHYLHEPTANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,4-DIMETHYLHEXANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,4-DIMETHYLOCTANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,4-DIMETHYLPENTANE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,5-DIMETHYLHEPTANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,5-DIMETHYLHEXANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,6-DIMETHYLOCTANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,6-DIMETHYLSTYRENE	1.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
2-BUTYLTETRAHYDROFURAN	0.00	6.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
2-BUTYNE	0.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
2-ETHYLHEXANOL	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-ETHYL-1-BUTENE	0.00	5.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00
2-ETHYL-1-HEXANOL	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-FURFURAL	1.00	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
2-HEXENE	0.00	2.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
2-METHYLDECANE	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-METHYLHEPTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-METHYLHEXANE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-METHYLOCTANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-METHYLPENTANE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-METHYLPROPANE	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-METHYLPROPENE	1.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-METHYLPROPENE	1.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-METHYL-1,3-BUTADIENE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00
2-METHYL-1-BUTENE	0.00	4.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00
2-METHYL-1-PENTENE	0.00	5.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00
2-METHYL-2-BUTENE	1.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-METHYL-2-PENTENE	1.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-METHYL-3-HEXANONE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-(2-BUTOXYETHOXY)-ETHANOL	0.00	4.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
3,3-DIMETHYLPENTANE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3,4-DIMETHYLOCTANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3,5,5-TRIMETHYLHEXANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3,5-DIMETHYLHEPTANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3-HEPTENE	0.00	3.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
3-METHYLHEPTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3-METHYLHEXANE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3-METHYLOCTANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3-METHYLPENTANE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3-METHYL-1-BUTENE	1.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3-METHYL-1-PENTENE	1.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
3-METHYL-CIS-2-PENTENE	1.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3-METHYL-TRANS-2-PENTENE	1.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3-(CHLOROMETHYL)-HEPTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4,4-METHYLENE DIANILINE	0.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	5.00
4-METHYLANILINE	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
4-METHYLHEPTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4-METHYLNONANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4-METHYLOCTANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4-METHYL-1-PENTENE	1.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4-METHYL-CIS-2-PENTENE	0.00	2.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
4-METHYL-TRANS-2-PENTENE	0.00	2.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
4-PHENYL-1-BUTENE	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
ACENAPHTHENE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	3.00
ACENAPHTHYLENE	1.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	2.00
ACETALDEHYDE	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
ACETIC ACID	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
ACETIC ANHYDRIDE	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
ACETONE	0.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETYLENE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
ACROLEIN (PROPENAL)	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00
ACRYLIC ACID	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
ACRYLONITRILE	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ADIPIC ACID	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
ALIPHATICS (per carbon)	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ALKENE KETONE	1.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AMINOANTHRAQUINONE	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	12.00
ANILINE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
ANTHANTHRENE	1.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	7.00
ANTHRACENE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	5.00
ANTHRAQUINONE	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	12.00
A-PINENE	0.50	6.00	0.00	0.00	0.00	1.50	0.00	0.00	0.00
BENZALDEHYDE	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	5.00
BENZENE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
BENZOIC ACID	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	6.00
BENZOPYRENES	1.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	3.00
BENZOTHIAZOLE	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
BENZO(a)ANTHRACENE	0.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	3.00
BENZO(a)PYRENE	1.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	3.00
BENZO(b)FLUORANTHENE	0.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	5.00
BENZO(c)PHENANTHRENE	0.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	3.00
BENZO(e)PYRENE	1.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	3.00
BENZO(g,h,i)FLUORANTHENE	0.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	3.00
BENZO(g,h,i)PERYLENE	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	6.00
BENZO(k)FLUORANTHENE	0.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	5.00
BENZYLCHLORIDE	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
BIPHENYL	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	5.00
BIPHENYLOL	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	5.00

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
BROMODINITROANILINE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
BROMODINITROBENZENE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
BUTENE	1.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
BUTOXYBUTENE	1.00	4.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
BUTOXYETHOXYETHANOL	0.00	4.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
BUTOXYETHOXYETHANOL ACETATE	0.00	5.00	0.00	0.00	0.00	2.00	0.00	0.00	1.00
BUTYL CARBITOL	0.00	4.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
BUTYL CELLOSOLVE	0.00	4.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
BUTYLACRYLATE	1.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
BUTYLBENZENE	0.00	3.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
BUTYLBENZOATE	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	6.00
BUTYLBENZYLPHTHALATE	0.00	5.00	1.00	0.00	0.00	0.00	0.00	0.00	7.00
BUTYLCYCLOHEXANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
BUTYLISOPROPYLPHTHALATE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	7.00
BUTYRALDEHYDE	0.00	2.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
B-PHELLANDRENE	2.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
B-PINENE	1.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C1 COMPOUNDS (DIESEL EXHAUST)	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.99
C10 AROMATIC	0.00	3.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C10 COMPOUNDS (DIESEL EXHAUST)	0.19	5.48	0.29	0.27	0.00	0.00	0.00	0.00	0.00
C10 OLEFINS	1.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C10 PARAFFINS	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C10H12	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
C10H16	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C10H16O	1.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C11 COMPOUNDS (DIESEL EXHAUST)	0.15	10.70	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C11 OLEFINS	1.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C11 PARAFFIN	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C11H10	0.00	3.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
C11H14O	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	1.00
C12 COMPOUNDS (DIESEL EXHAUST)	0.00	5.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C12 OLEFINS	1.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C12 PARAFFIN	0.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C12H22	0.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C13 COMPOUNDS (DIESEL EXHAUST)	0.00	6.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C13 PARAFFIN	0.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C14 COMPOUNDS (DIESEL EXHAUST)	0.00	7.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C15 COMPOUNDS (DIESEL EXHAUST)	0.00	8.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C16 BRANCHED ALKANE	0.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C16 COMPOUNDS (DIESEL EXHAUST)	0.00	9.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C17 COMPOUNDS (DIESEL EXHAUST)	0.00	10.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C18 COMPOUNDS (DIESEL EXHAUST)	0.00	11.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C19 COMPOUNDS (DIESEL EXHAUST)	0.00	12.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C2 ALKYLANTHRACENES	0.00	3.00	0.00	1.00	0.00	0.00	0.00	0.00	5.00
C2 ALKYLBENZANTHRACENE	0.00	2.00	1.00	1.00	0.00	0.00	0.00	0.00	3.00
C2 ALKYLBENZOPHENANTHRENE	0.00	2.00	1.00	1.00	0.00	0.00	0.00	0.00	3.00
C2 ALKYLCHRYSENES	0.00	2.00	1.00	1.00	0.00	0.00	0.00	0.00	3.00

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
C2 ALKYLCYCLOHEXANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C2 ALKYLINDAN	0.00	3.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
C2 ALKYLNAPTHALENE	0.00	4.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
C2 ALKYLPHENANTHRENES	0.00	3.00	0.00	1.00	0.00	0.00	0.00	0.00	5.00
C2 COMPOUNDS (DIESEL EXHAUST)	0.00	0.77	0.00	0.00	0.00	0.00	0.12	0.00	1.00
C20 COMPOUNDS (DIESEL EXHAUST)	0.00	13.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C21 COMPOUNDS (DIESEL EXHAUST)	0.00	14.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C22 COMPOUNDS (DIESEL EXHAUST)	0.00	15.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C23 COMPOUNDS (DIESEL EXHAUST)	0.00	16.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C24 COMPOUNDS (DIESEL EXHAUST)	0.00	17.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C25 COMPOUNDS (DIESEL EXHAUST)	0.00	18.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C26 COMPOUNDS (DIESEL EXHAUST)	0.00	19.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C27 COMPOUNDS (DIESEL EXHAUST)	0.00	20.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C28 COMPOUNDS (DIESEL EXHAUST)	0.00	21.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C29 COMPOUNDS (DIESEL EXHAUST)	0.00	22.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C3 ALKYLCYCLOHEXANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C3 ALKYLSTYRENE	1.00	2.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C3 COMPOUNDS (DIESEL EXHAUST)	0.90	1.07	0.00	0.00	0.00	0.00	0.00	0.00	0.12
C3 PARAFFIN	0.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C30 COMPOUNDS (DIESEL EXHAUST)	0.00	23.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C31 COMPOUNDS (DIESEL EXHAUST)	0.00	24.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C32 COMPOUNDS (DIESEL EXHAUST)	0.00	25.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C33 COMPOUNDS (DIESEL EXHAUST)	0.00	26.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C34 COMPOUNDS (DIESEL EXHAUST)	0.00	27.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C35 COMPOUNDS (DIESEL EXHAUST)	0.00	28.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C36 COMPOUNDS (DIESEL EXHAUST)	0.00	29.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C37 COMPOUNDS (DIESEL EXHAUST)	0.00	30.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C38 COMPOUNDS (DIESEL EXHAUST)	0.00	31.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C39 COMPOUNDS (DIESEL EXHAUST)	0.00	32.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C3/C4/C5 ALKYLBENZENES	0.00	3.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C4 ALKYLPHENOLS	0.00	3.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C4 ALKYLSTYRENES	1.00	3.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C4 COMPOUNDS (DIESEL EXHAUST)	0.04	3.70	0.00	0.00	0.00	0.11	0.00	0.00	0.00
C4 OLEFIN	1.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C4 PARAFFIN	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C4 SUBSTITUTED CYCLOHEXANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C4 SUBSTITUTED CYCLOHEXANONE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C40 COMPOUNDS (DIESEL EXHAUST)	0.00	33.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C41 COMPOUNDS (DIESEL EXHAUST)	0.00	34.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C42 COMPOUNDS (DIESEL EXHAUST)	0.00	35.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C43 COMPOUNDS (DIESEL EXHAUST)	0.00	36.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C5 ALKYL CYCLOHEXANE	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C5 ALKYLBENZENES	0.00	4.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C5 ALKYLBENZENES (UNSATURATED)	1.00	2.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C5 ALKYLPHENOLS	0.00	4.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C5 COMPOUNDS (DIESEL EXHAUST)	0.04	4.60	0.00	0.00	0.00	0.15	0.00	0.00	0.00
C5 ESTER	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
C5 OLEFIN	1.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C5 PARAFFIN	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C5 PARAFFIN/OLEFIN	0.50	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C5 SUBSTITUTED CYCLOHEXANE	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C5H10O	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C6 ALKYLBENZENE	0.00	5.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C6 COMPOUNDS (DIESEL EXHAUST)	0.22	4.50	0.00	0.00	0.00	0.07	0.00	0.00	0.93
C6 OLEFINS	1.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C6 PARAFFIN	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C6 SUBSTITUTED CYCLOHEXANE	0.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C6H18O3SI3	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C7 ALKYLBENZENE	0.00	6.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C7 COMPOUNDS (DIESEL EXHAUST)	0.00	1.40	0.80	0.00	0.00	0.00	0.00	0.00	0.00
C7 CYCLOPARAFFINS	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C7 OLEFINS	1.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C7 PARAFFINS	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C7H12	1.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C7H12O	1.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C7-C16	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C8 COMPOUNDS (DIESEL EXHAUST)	0.21	4.90	0.00	0.34	0.00	0.00	0.00	0.00	0.00
C8 CYCLOPARAFFINS	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C8 OLEFINS	1.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C8 PARAFFIN	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C8 PHENOLS	0.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
C8H14	1.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C8H24O4SI4	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C9 COMPOUNDS (DIESEL EXHAUST)	0.00	3.62	0.06	0.61	0.00	0.06	0.00	0.00	0.00
C9 CYCLOPARAFFINS	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C9 OLEFINS	1.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C9 PARAFFIN	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C9 PHENOLS	0.00	2.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
CAMPHENE	1.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CAPROLACTAM	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
CARBITOL	0.00	2.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
CARBON DISULFIDE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CARBON TETRACHLORIDE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
CARBONYL SULFIDE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
CARYOPHYLLENE	3.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CELLOSOLVE	0.00	2.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
CELLOSOLVE ACETATE	0.00	3.00	0.00	0.00	0.00	1.00	0.00	0.00	1.00
CHLOROBENZENE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
CHLORODIFLUOROMETHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
CHLOROFORM	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
CHLOROPENTAFLUOROETHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
CHLOROPRENE	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CHLOROTRIFLUOROMETHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
CHRYSENE	0.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	3.00

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
CIS-1,4-DIMETHYLCYCLOHEXANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CIS-2-BUTENE	0.00	0.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
CIS-2-HEPTENE	0.00	3.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
CIS-2-HEXENE	0.00	2.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
CIS-2-OCTENE	0.00	4.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
CIS-2-PENTENE	0.00	1.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
CIS-3-HEXENE	0.00	2.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
CORONENE	0.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	9.00
CREOSOTE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	2.00
CRESOL	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
CROTONALDEHYDE	1.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
CUMENE (ISOPROPYL BENZENE)	0.00	2.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
CYCLOHEPTANE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CYCLOHEXANE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CYCLOHEXANOL	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CYCLOHEXANONE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CYCLOHEXENE	0.00	2.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
CYCLOPENTAANTHRACENES	0.00	3.00	0.00	1.00	0.00	0.00	0.00	0.00	5.00
CYCLOPENTANE	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CYCLOPENTAPHENANTHRENES	0.00	3.00	0.00	1.00	0.00	0.00	0.00	0.00	5.00
CYCLOPENTA(c,d)PYRENE	0.00	2.00	1.00	1.00	0.00	0.00	0.00	0.00	1.00
CYCLOPENTENE	0.00	1.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
CYCLOPENTYLCYCLOPENTANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DECALINS	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DENATURANT	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIACETONE ALCOHOL	0.00	4.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
DIBENZANTHRACENES	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	6.00
DIBENZOPYRENES	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	8.00
DIBENZO(a,h)ANTHRACENE	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	6.00
DIBENZPHENANTHRENES	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	6.00
DIBUTYL ETHER	0.00	6.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
DIBUTYLPHTHALATE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	7.00
DICHLOROBENZENES	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
DICHLORODIFLUOROMETHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
DICHLOROMETHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
DICHOLROTETRAFLUOROETHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
DIETHYLCYCLOHEXANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIETHYLENE GLYCOL	0.00	2.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
DIETHYLMETHYLCYCLOHEXANE	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIHYDRONAPTHALENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
DIHYDROXYNAPTHALENEDIONE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
DIISOPROPYLBENZENE	0.00	4.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
DIMETHYL ALKYL AMINES	0.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLBENZYLALCOHOL	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLBUTANE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLBUTANEDIOATE	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
DIMETHYLBUTENE	1.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
DIMETHYLBUTYLCYCLOHEXANE	0.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLCYCLOBUTANONE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLCYCLOHEXANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLCYCLOPENTANE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLCYCLOPENTENES	1.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLDECANE	0.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLETHER	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLETHYLBENZOIC ACID	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	1.00
DIMETHYLETHYLCYCLOHEXANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLFORMAMIDE	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
DIMETHYLHEPTANES	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLHEPTANOL	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLHEXADIENE	1.00	2.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
DIMETHYLHEXANEDIOATE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
DIMETHYLHEXANES	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLHEXENE	1.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLINDANS	0.00	3.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLINDENE	1.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLNAPHTHYRIDINE	0.00	3.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLNAPTHALENE	0.00	4.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLNONANES	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLOCTANES	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLOCTANOL	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLOCTENES	1.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLOCTYNE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
DIMETHYLPENTANE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLPENTANEDIOATE	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
DIMETHYLPENTANOL	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLPENTENE	1.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIMETHYLPHTHALATE	0.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	7.00
DIMETHYLTEREPHTHALATE	0.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	7.00
DIMETHYLUNDECANE	0.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DIPHENYLETHANE	0.00	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00
DIPROPYLENE GLYCOL	0.00	4.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
DIPROPYLPHTHALATE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	7.00
DIVINYLBENZENE	1.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
DI(ETHYLPHENYL)ETHANE	0.00	4.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00
DI-C8 ALKYL PHTHALATE	0.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	7.00
DODECENE	1.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
D-LIMONENE	1.00	4.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
EICOSANE	0.00	20.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
EPICHLOROHYDRIN	0.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHANE	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	1.60
ETHANOLAMINE	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	1.60
ETHYL ACETATE	0.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
ETHYL ACRYLATE	1.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
ETHYL ALCOHOL	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	1.60

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
ETHYL CHLORIDE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
ETHYL ETHER	0.00	2.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
ETHYLAMINE	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	1.60
ETHYLBENZENE	0.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLBICYCLOHEPTANE	0.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLCYCLOHEXANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLCYCLOPENTANE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLCYCLOPENTENE	1.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLDIMETHYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
ETHYLDIMETHYLCYCLOHEXANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLDIMETHYLOCTANE	0.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLDIMETHYLPENTANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLDIMETHYLPHENOL	0.00	2.00	0.00	1.00	0.00	0.00.	0.00	0.00	0.00
ETHYLENE	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
ETHYLENE DIBROMIDE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
ETHYLENE DICHLORIDE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
ETHYLENE GLYCOL	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	1.60
ETHYLENE OXIDE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
ETHYLENEAMINES	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	1.60
ETHYLFURAN	2.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLHEPTANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLHEPTENE	1.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLHEXANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLHEXANOATE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
ETHYLINDAN	0.00	3.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
ETHYLISOPROPYL ETHER	0.00	3.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
ETHYLMERCAPTAN	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLMETHYLCYCLOHEXANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLMETHYLCYCLOPENTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLMETHYLHEXANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLMETHYLOCTANE	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLOCTANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLOCTENE	1.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLPENTENE	1.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLPHENYLPHENYLETHANE	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00
ETHYLPROPYLCYCLOHEXANE	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLSTYRENE	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLTOLUENE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
ETHYL-T-BUTYL ETHER	0.00	4.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
FLUORANTHENE	0.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	1.00
FLUORENE	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	5.00
FORMALDEHYDE	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00
FORMIC ACID	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
FURFURYL ALCOHOL	2.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
GLYCEROL	0.00	1.50	0.00	0.00	0.00	0.00	0.00	0.00	1.50
GLYCOL	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	1.60
GLYCOL ETHER	0.00	0.80	0.00	0.00	0.00	0.00	0.00	0.00	3.20

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
GLYOXAL	0.00	1.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00
HENEICOSANE	0.00	21.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HEPTADIENAL	1.00	1.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
HEPTANE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HEPTANONE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HEPTENE	1.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HEXADECANE	0.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HEXADECANOIC ACID	0.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
HEXADIENAL	1.00	0.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
HEXAFLUOROETHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
HEXAMETHYLENEDIAMINE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HEXANAL	0.00	4.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
HEXANE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HEXENE	1.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HEXYLENE GLYCOL	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HEXYNE	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
INDANE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
INDENE	0.50	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
INDENO(1,2,3-cd)PYRENE	1.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	4.00
ISOAMYL ALCOHOL	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOAMYLBENZENE	0.00	4.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOBUTANE	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOBUTYL ALCOHOL	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOBUTYLACETATE	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
ISOBUTYLACRYLATE	1.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
ISOBUTYLBENZENE	0.00	3.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOBUTYLENE	1.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOBUTYLISOBUTYRATE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
ISOBUTYRALDEHYDE	0.00	2.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
ISOMERS OF BUTENE	1.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF BUTYLBENZENE	0.00	3.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF C10H10	1.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF C10H18	1.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF C11H20	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF C9H16	1.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF DECANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF DIETHYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF DODECANE	0.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF ETHYLTOLUENE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF HEPTADECANE	0.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF HEPTANE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF HEXANE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF NONANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF OCTADECANE	0.00	18.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF OCTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF PENTADECANE	0.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF PENTANE	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
ISOMERS OF PENTENE	1.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF PROPYLBENZENE	0.00	2.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF TETRADECANE	0.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF TRIDECANE	0.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF UNDECANE	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOMERS OF XYLENE	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
ISOOCTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOPENTANE	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOPRENE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00
ISOPROPYL ALCOHOL	0.00	1.50	0.00	0.00	0.00	0.00	0.00	0.00	1.50
ISOPROPYLACETATE	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
ISOPROPYLBENZENE	0.00	2.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOPROPYLCYCLOHEXANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOPROPYLCYCLOPENTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOPROPYLMETHYLCYCLOHEXANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ISOVALERALDEHYDE	0.00	3.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
LACTOL SPIRITS	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LIMONENE	1.00	4.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
MALEIC ANHYDRIDE	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHOXYETHOXYBUTANONE	0.00	5.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
METHOXYETHOXYETHANOL	0.00	3.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
METHOXYNAPHTHALENE	0.00	3.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
METHYL ALCOHOL	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYL C11 ESTER	0.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYL C12 ESTER	0.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYL C13 ESTER	0.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYL C14 ESTER	0.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYL C15 ESTER	0.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYL C19 ESTER	0.00	20.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYL C20 ESTER	0.00	21.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLACETATE	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLACETOPHENONE	0.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLACETYLENE (PROPYNE)	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLACRYLATE	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLAL	0.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLALLENE	1.50	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLAMYL KETONE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLANTHRACENES	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	5.00
METHYLBENZANTHRACENES	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	3.00
METHYLBENZPHENANTHRENE	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	3.00
METHYLBIPHENYL	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	5.00
METHYLBUTADIENE	2.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLBUTENE	1.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLBUTYL KETONE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLCARBITOL	0.00	3.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
METHYLCELLOSOLVE	0.00	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
METHYLCHLORIDE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLCHRYSENES	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	3.00
METHYLCYCLOHEXADIENE	1.00	1.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
METHYLCYCLOHEXANE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLCYCLOHEXENE	1.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLCYCLOOCTANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLCYCLOPENTADIENE	1.00	0.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
METHYLCYCLOPENTANE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLCYCLOPENTENE	1.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLDECALINS	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLDECANES	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLDECENE	1.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLDIHYDRONAPHTHALE	0.00	3.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
METHYLDODECANE	0.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLDODECANOATE	0.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLENE BROMIDE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLENE CHLORIDE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLENEBIS(C6H4NCO)	0.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	7.00
METHYLENE(b)4-PHENYLISOCYANATE	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	8.00
METHYLETHYL KETONE	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLETHYLHEPTANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLETHYLPENTANOATE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLFLUORANTHENES	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	1.00
METHYLFORMATE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLGLYOXAL	0.00	0.00	0.00	0.00	1.00	1.00	0.00	0.00	0.00
METHYLHEPTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLHEPTANOL	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLHEPTENE	1.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLHEPTYNE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLHEXADIENE	1.00	1.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
METHYLHEXANAL	0.00	5.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
METHYLHEXANE	0.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLHEXENES	1.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLINDANS	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
METHYLINDENE	1.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
METHYLISOBUTYL KETONE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLISOPROPYLCYCLOHEXANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLMETHACRYLATE	1.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLMETHYLPROPENOATE	1.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLMYRISTATE	0.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLNAPHTHALENES	0.00	3.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
METHYLNONANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLNONENE	1.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLOCTANES	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLPALMITATE	0.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLPENTANE	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLPENTENES	1.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
METHYLPHENANTHRENES	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	5.00
METHYLPROPYLCYCLOHEXANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLPROPYLNONANE	0.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLSTEARATE	0.00	18.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
METHYLSTYRENE	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYLUNDECANE	0.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHYL-T-BUTYL ETHER	0.00	3.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
MINERAL SPIRITS	0.00	6.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
MYRCENE	3.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
M-DICHLOROBENZENE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
M-DIETHYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
M-ETHYLTOLUENE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
M-XYLENE	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
M-XYLENE AND P-XYLENE	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
NAPHTHA	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
NAPTHALENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
NITROBENZENE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
NONADECANE	0.00	19.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
NONADIENE	1.00	3.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
NONANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
NONENE	1.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
NONENONE	1.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
NONYLPHENOL	0.00	8.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
N-AMYLBENZENE	0.00	4.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
N-BUTANE	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-BUTYL ALCOHOL	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-BUTYLACETATE	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
N-DECANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-DODECANE	0.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-HEPTADECANE	0.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-HEXYLBENZENE	0.00	5.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
N-PENTADECANE	0.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-PENTANE	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-PENTENE	1.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-PENTYLCYCLOHEXANE	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-PHENYLANILINE	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	5.00
N-PROPYL ALCOHOL	0.00	1.50	0.00	0.00	0.00	0.00	0.00	0.00	1.50
N-PROPYLACETATE	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
N-PROPYLBENZENE	0.00	2.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
N-TETRADECANE	0.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-TRIDECANE	0.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-UNDECANE	0.00	11,00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OCTAHYDROINDENES	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OCTAMETHYLCYCLOTETRASILOXANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OCTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OCTANOL	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OCTATRIENE	2.00	0.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
OCTENE	1.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OXYGENATES	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
O-DICHLOROBENZENE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
O-ETHYLTOLUENE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
O-XYLENE	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
PALMITIC ACID	0.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
PARAFFINS (C16-C34)	0.00	25.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PARAFFINS (C2-C7)	0.00	4.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PARAFFINS/OLEFINS (C12-C16)	0.50	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PENTADIENE	2.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PENTANOL	0.00	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PENTENYNE	1.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
PENTYLBENZENE	0.00	4.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
PENTYLCYCLOHEXANE	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PENTYLIDENECYCLOHEXANE	1.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PENTYNE	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
PERCHLOROETHYLENE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
PERYLENE	0.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	5.00
PHENANTHRENE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	5.00
PHENOL	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
PHENYLISOCYANATE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	6.00
PHENYLNAPHTHALENES	0.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00
PHTHALIC ANHYDRIDE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	7.00
PIPERYLENE	2.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
POLYETHYLENE GLYCOL	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PROPADIENE	1.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PROPANE	0.00	1.50	0.00	0.00	0.00	0.00	0.00	0.00	1.50
PROPENE	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PROPENYLCYCLOHEXANE	1.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PROPIONALDEHYDE	0.00	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
PROPIONIC ACID	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
PROPYLBENZENE	0.00	2.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
PROPYLCYCLOHEXANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PROPYLENE DICHLORIDE	0.00	1.50	0.00	0.00	0.00	0.00	0.00	0.00	1.50
PROPYLENE GLYCOL	0.00	1.50	0.00	0.00	0.00	0.00	0.00	0.00	1.50
PROPYLENE OXIDE	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
PROPYLHEPTENES	1.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PYRENE	0.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	1.00
P-DICHLOROBENZENE	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
P-ETHYLTOLUENE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
P-TOLUALDEHYDE	0.00	0.00	0.00	0.00	0.00	2.00	0.00	0.00	4.00
P-XYLENE	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
SEC-BUTYL ALCOHOL	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SEC-BUTYLBENZENE	0.00	3.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
SILOXANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
STYRENE	0.50	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
SUBSTITUTED C9 ESTER (C12)	0.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
TEREPHTHALIC ACID	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	7.00
TERPENES	1.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TETRACHLOROBENZENES	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
TETRAFLUOROMETHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
TETRAMETHYLBENZENE	0.00	2.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
TETRAMETHYLCYCLOBUTENE	1.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TETRAMETHYLCYCLOPENTANE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TETRAMETHYLHEXANE	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TETRAMETHYLPENTANONE	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TETRAMETHYLSILANE	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TETRAMETHYLTHIOUREA	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
TOLUENE	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
TOLUENE DIISOCYANATE	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	2.00
TOLUENE ISOCYANATE	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	1.00
TOTAL AROMATIC AMINES	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
TOTAL C2-C5 ALDEHYDES	0.00	1.50	0.00	0.00	0.00	1.00	0.00	0.00	0.00
TRANS-1-PHENYLBUTENE	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
TRANS-2-BUTENE	0.00	0.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
TRANS-2-HEPTENE	0.00	3.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
TRANS-2-HEXENE	0.00	2.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
TRANS-2-NONENE	0.00	5.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
TRANS-2-PENTENE	0.00	1.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
TRANS-3-HEXENE	0.00	2.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
TRICHLOROBENZENES	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	5.00
TRICHLOROFLUOROMETHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
TRICHLOROTRIFLUOROETHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00
TRICHOLROETHYLENE	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
TRIETHYLENE GLYCOL	0.00	2.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
TRIFLUOROMETHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
TRIMETHYLAMINE	0.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLBENZENE	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLCYCLOHEXANES	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLCYCLOHEXANOL	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLCYCLOPENTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLCYCLOPENTANONE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLDECANE	0.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLDECENE	1.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLFLUOROSILANE	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
TRIMETHYLHEPTANES	0.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLHEXANES	0.00	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLHEXENE	1.00	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLINDAN	0.00	4.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLNONENE	1.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLOCTANES	0.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLPENTADIENE	2.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TRIMETHYLPENTANE	0.00	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
T-BUTYL ALCOHOL	0.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

TABLE B-2

SPECIES PROFILES BY BOND GROUPS FOR CB-4

CHEMICAL NAME	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
T-BUTYLBENZENE	0.00	2.00	1.00	0.00	0.00	0.00	0.00	0.00	1.00
UNIDENTIFIED	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
VINYL ACETATE	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
VINYL CHLORIDE	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
XYLENE BASE ACIDS	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00

APPENDIX C

TEST CASE RUN OUTPUT

```
****************************************
*                                      *
*   OZONE ISOPLETH PLOTTING PACKAGE    *
*     WITH OPTIONAL MECHANISMS         *
*                                      *
*           O Z I P M - 4              *
*                                      *
*             MAY, 1989                *
*                                      *
****************************************
```

```
TEST CASE


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

        LOS ANGELES, CALIF.

LATITUDE    34.058

LONGITUDE  118.250

TIME ZONE   7.0

DATE        6    21   1986

TIME        800  TO   1800    LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS    INITIAL  510.    FINAL      630.

TIMING               START    800.    STOP      1500.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME      800     900    1000    1100    1200    1300    1400    1500

HEIGHT    510.0   530.9   557.3   582.0   600.2   613.1   622.6   630.0

REACTIVITY

EMISSIONS       ETH  FRACTION 0.037   OLE  FRACTION 0.035   ALD2 FRACTION 0.052

EMISSIONS       FORM FRACTION 0.021   TOL  FRACTION 0.089   XYL  FRACTION 0.117

EMISSIONS       PAR  FRACTION 0.564   NR   FRACTION 0.085

NO2/NOX      0.250
```

```
                         TEST CASE

 TIME     NMOC      NMOC/       NOX       NO2        O3
(LDT )    TOTAL      NOX       TOTAL    FRACTION  (INSTANT)

 800.    1.00000   10.00000   0.10000   0.25000   0.00000

 900.    0.93318   10.11670   0.09224   0.45350   0.01249

1000.    0.84563   10.78440   0.07841   0.72144   0.04464

1100.    0.76023   12.77614   0.05950   0.84197   0.09786

1200.    0.67940   18.13698   0.03746   0.89870   0.16365

1300.    0.59977   37.94343   0.01581   0.93430   0.23743

1400.    0.53808  133.97348   0.00402   0.95470   0.28547

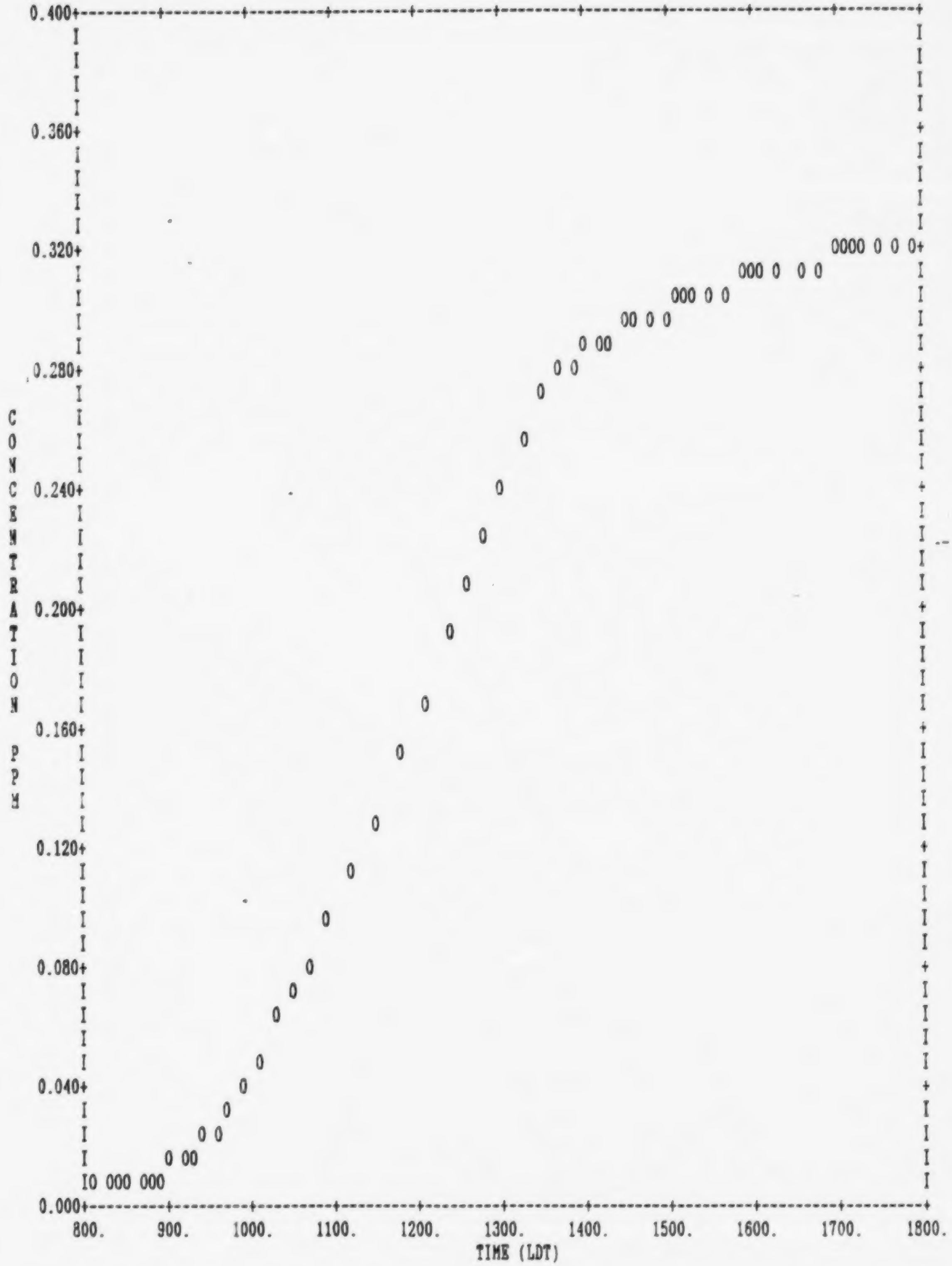
1500.    0.50054  227.14540   0.00220   0.96107   0.29914

1600.    0.47674  225.09323   0.00212   0.96380   0.30931

1700.    0.45927  204.30595   0.00225   0.96775   0.31735

1800.    0.44836  176.18916   0.00254   0.97503   0.32322

               MAXIMUM ONE HOUR AVE O3    = 0.32048 CENTERED AT 1730. LDT
```


0.400
0.360
0.320
0.280
0.240
0.200
0.160
0.120
0.080
0.040
0.000
CONCENTRATION PPM
800.
900.
1000.
1100.
1200.
1300.
1400.
1500.
1600.
1700.
1800.
TIME (LDT)

TEST CASE

APPENDIX D

EXAMPLE OF SINGLE CALCULATION OUTPUT

```
****************************************
*                                      *
*  OZONE ISOPLETH PLOTTING PACKAGE     *
*    WITH OPTIONAL MECHANISMS          *
*                                      *
*          O Z I P M - 4               *
*                                      *
*           MAY, 1989                  *
*                                      *
****************************************
```

```
EXAMPLE OF SINGLE CALCULATION


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR


       TEST CITY


LATITUDE    38.629

LONGITUDE   90.206

TIME ZONE   6.0

DATE        6    21   1988

TIME        800  TO   1800    LOCAL DAYLIGHT TIME



DILUTION.DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS    INITIAL  250.    FINAL     1700.

TIMING               START    800.    STOP      1500.



MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME       800     900    1000    1100    1200    1300    1400    1500

HEIGHT     250.0   503.1  821.2   1119.5  1340.2  1496.2  1610.8  1700.0



TEMPERATURE (AT THE BEGINNING OF EACH HOUR)

HOUR       0      1      2      3      4      5      6      7      8      9
           10     11

TEMP       294.0  296.0  299.0  301.0  304.0  305.0  307.0  308.0  306.0  305.0
           304.0  302.0



RELATIVE HUMIDITY (AT THE BEGINNING OF EACH HOUR)

HOUR       0      1      2      3      4      5      6      7      8      9
           10     11

RH (%)     80.0   75.0   50.0   45.0   40.0   35.0   30.0   30.0   30.0   30.0
           35.0   40.0
```

```
TRANSPORTED CONCENTRATIONS

ALOFT               OZONE   0.040     HYDROCARBON  0.030    NOX     0.002 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)

SPECIES     HOUR          1     2     3     4     5     6     7     8     9    10
                         11

 VOC      FRACTION     0.079 0.065 0.063 0.044 0.027 0.019 0.018 0.015 0.014 0.018
                       0.009

 NOX      FRACTION     0.215 0.163 0.149 0.109 0.073 0.050 0.051 0.042 0.038 0.047
                       0.024

 CO       FRACTION     0.038 0.056 0.041 0.034 0.034 0.034 0.034 0.036 0.041 0.045
                       0.060


TRANSPORTED BIOGENIC CONCENTRATIONS


SURFACE LAYER        ISOP    0.000     APIN         0.000

ALOFT                ISOP    0.000     APIN         0.000


THE FOLLOWING BIOGENIC SPECIES ARE TREATED AS HYDROCARBONS
(EXPRESSED AS BOND FRACTIONS)

APIN            ETH  FRACTION 0.000   OLE  FRACTION 0.500   ALD2 FRACTION 1.500
                FORM FRACTION 0.000   TOL  FRACTION 0.000   XYL  FRACTION 0.000
                PAR  FRACTION 6.000   NR   FRACTION 0.000


BIOGENIC EMISSIONS (IN UNITS OF PPM/HR)

SPECIES     HOUR          1     2     3     4     5     6     7     8     9    10
                         11

 ISOP                  0.000 0.000 0.000 0.000 0.001 0.001 0.002 0.002 0.001 0.001
                       0.001

 APIN                  0.000 0.000 0.000 0.000 0.001 0.001 0.002 0.001 0.001 0.001
                       0.001
```

```
WATER CONCENTRATIONS (AT THE BEGINNING OF EACH HOUR)

HOUR        0      1      2      3      4      5      6      7      8      9
           10     11

PPM      19333.  20417.  16210.  18349.  17176.  15875.  15159.  15989.  14366.  13607.
         15029.  15373.

PRESSURE      29.95 INCHES OF HG


REACTIVITY

EMISSIONS       ETH  FRACTION 0.037   OLE  FRACTION 0.035   ALD2 FRACTION 0.052

EMISSIONS       FORM FRACTION 0.021   TOL  FRACTION 0.089   XYL  FRACTION 0.117

EMISSIONS       PAR  FRACTION 0.564   NR   FRACTION 0.085

ALOFT           ETH  FRACTION 0.034   OLE  FRACTION 0.020   ALD2 FRACTION 0.037

ALOFT           FORM FRACTION 0.070   TOL  FRACTION 0.042   XYL  FRACTION 0.026

ALOFT           PAR  FRACTION 0.498   NR   FRACTION 0.273

NO2/NOX      0.250
```

```
                          EXAMPLE OF SINGLE CALCULATION

 TIME     NMOC       NMOC/       NOX        NO2         O3
(LDT )    TOTAL      NOX         TOTAL      FRACTION    (INSTANT)

  800.   0.80010   10.00125    0.08000    0.25000    0.00000

  900.   0.42922    9.20272    0.04664    0.52956    0.02159

 1000.   0.27629    9.34275    0.02957    0.67070    0.03988

 1100.   0.20770   10.23478    0.02029    0.74582    0.05704

 1200.   0.16933   12.69081    0.01334    0.81436    0.07892

 1300.   0.14184   19.44312    0.00729    0.87057    0.10678

 1400.   0.12207   32.36849    0.00377    0.90964    0.13198

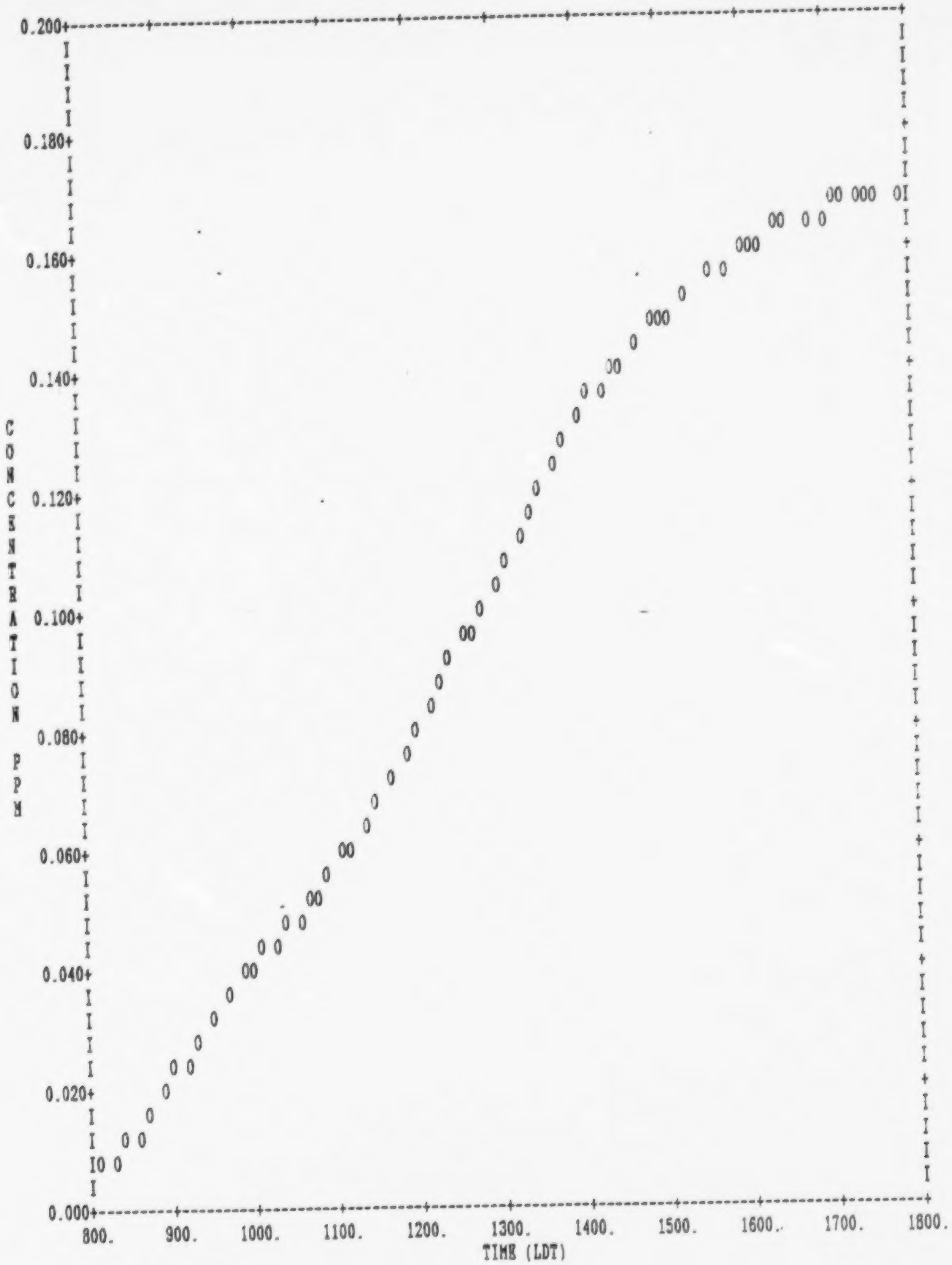
 1500.   0.11028   39.21800    0.00281    0.92456    0.14755

 1600.   0.10581   45.15876    0.00234    0.93231    0.15965

 1700.   0.10408   47.18596    0.00221    0.94540    0.16583

 1800.   0.10468   42.13735    0.00248    0.96803    0.16826

                 MAXIMUM ONE HOUR AVE O3    = 0.16730 CENTERED AT 1730. LDT
```



EXAMPLE OF SINGLE CALCULATION

APPENDIX E

EXAMPLE OF EKMA OPTION OUTPUT

```
***************************************
*                                     *
*   OZONE ISOPLETH PLOTTING PACKAGE   *
*      WITH OPTIONAL MECHANISMS       *
*                                     *
*             O Z I P M - 4           *
*                                     *
*               MAY, 1989             *
*                                     *
***************************************
```

```
EXAMPLE OF EKMA OPTION


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

         TEST CITY

LATITUDE     38.629

LONGITUDE    90.206

TIME ZONE    6.0

DATE         6     21    1988

TIME         800   TO    1800     LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS     INITIAL  250.     FINAL      1700.

TIMING                START    800.     STOP       1500.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME       800     900     1000    1100    1200    1300    1400    1500

HEIGHT     250.0   503.1   821.2   1119.5  1340.2  1496.2  1610.8  1700.0


TEMPERATURE (AT THE BEGINNING OF EACH HOUR)

HOUR         0       1       2       3       4       5       6       7       8       9
            10      11

TEMP       294.0   296.0   299.0   301.0   304.0   305.0   307.0   308.0   306.0   305.0
           304.0   302.0


RELATIVE HUMIDITY (AT THE BEGINNING OF EACH HOUR)

HOUR         0       1       2       3       4       5       6       7       8       9
            10      11

RH (%)      80.0    75.0    50.0    45.0    40.0    35.0    30.0    30.0    30.0    30.0
            35.0    40.0
```

```
WATER CONCENTRATIONS (AT THE BEGINNING OF EACH HOUR)

HOUR        0      1      2      3      4      5      6      7      8      9
           10     11

PPM       19333. 20417. 16210. 16349. 17176. 15875. 15159. 15989. 14366. 13607.
          15029. 15373.

PRESSURE     29.95 INCHES OF HG


REACTIVITY

EMISSIONS       ETH  FRACTION 0.037   OLE  FRACTION 0.035   ALD2 FRACTION 0.052

EMISSIONS       FORM FRACTION 0.021   TOL  FRACTION 0.089   XYL  FRACTION 0.117

EMISSIONS       PAR  FRACTION 0.564   NR   FRACTION 0.085

ALOFT           ETH  FRACTION 0.034   OLE  FRACTION 0.020   ALD2 FRACTION 0.037

ALOFT           FORM FRACTION 0.070   TOL  FRACTION 0.042   XYL  FRACTION 0.026

ALOFT           PAR  FRACTION 0.498   NR   FRACTION 0.273

NO2/NOX      0.250
```

```
TRANSPORTED CONCENTRATIONS

ALOFT               OZONE    0.040     HYDROCARBON  0.030    NOX     0.002 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)

SPECIES    HOUR          1     2     3     4     5     6     7     8     9    10
                        11

  VOC     FRACTION     0.099 0.081 0.079 0.055 0.034 0.024 0.023 0.018 0.018 0.022
                       0.012

  NOX     FRACTION     0.215 0.163 0.149 0.109 0.073 0.050 0.051 0.042 0.038 0.047
                       0.024

  CO      FRACTION     0.038 0.056 0.041 0.034 0.034 0.034 0.034 0.038 0.041 0.045
                       0.060


TRANSPORTED BIOGENIC CONCENTRATIONS


SURFACE LAYER       ISOP    0.000     APIN        0.000

ALOFT               ISOP    0.000     APIN        0.000


THE FOLLOWING BIOGENIC SPECIES ARE TREATED AS HYDROCARBONS
(EXPRESSED AS BOND FRACTIONS)

APIN           ETH  FRACTION 0.000   OLE  FRACTION 0.500   ALD2 FRACTION 1.500
               FORM FRACTION 0.000   TOL  FRACTION 0.000   XYL  FRACTION 0.000
               PAR  FRACTION 6.000   NR   FRACTION 0.000


BIOGENIC EMISSIONS (IN UNITS OF PPM/HR)

SPECIES    HOUR          1     2     3     4     5     6     7     8     9    10
                        11

  ISOP                 0.000 0.000 0.000 0.000 0.001 0.001 0.002 0.002 0.001 0.001
                       0.001

  APIN                 0.000 0.000 0.000 0.000 0.001 0.001 0.002 0.001 0.001 0.001
                       0.001
```

```
EKMA CALCULATIONS ARE PERFORMED TO ESTIMATE

SITE-SPECIFIC VOC CONTROL REQUIREMENTS

BASE YEAR OZONE                           0.150 PPM

BASE YEAR NMOC/NOX                        8.000

ANTICIPATED CHANGE IN NOX               -10.000 PERCENT

FUTURE OZONE TRANSPORTED ALOFT            0.040 PPM

FUTURE NMOC TRANSPORTED ALOFT             0.024 PPMC

FUTURE NOX TRANSPORTED ALOFT              0.002 PPM

EMISSION CREDITS WILL BE ALLOWED FOR CO

ANTICIPATED CHANGE IN CO                -50.000 PERCENT

FUTURE CO   TRANSPORTED ALOFT             0.500 PPM

FUTURE BIOGENIC EMISSIONS WILL BE SET FOR ISOP

ANTICIPATED CHANGE IN ISOP                0.000 PERCENT

FUTURE ISOP TRANSPORTED IN THE SURFACE LAYER     0.000 PPM

FUTURE ISOP TRANSPORTED ALOFT             0.000 PPM

FUTURE BIOGENIC EMISSIONS WILL BE SET FOR APIN

ANTICIPATED CHANGE IN APIN                0.000 PERCENT

FUTURE APIN TRANSPORTED IN THE SURFACE LAYER     0.000 PPM

FUTURE APIN TRANSPORTED ALOFT             0.000 PPM

FUTURE OZONE IN THE SURFACE LAYER         0.000 PPM

FUTURE NMOC IN THE SURFACE LAYER          0.000 PPMC

FUTURE NOX IN THE SURFACE LAYER           0.000 PPM
```

```
                    THE FOLLOWING SIMULATIONS WERE DONE.

   NMOC          NOX          RATIO          O3          TIME

  1.00000      0.12500      8.00000      0.18133      NOT MAX

  0.82720      0.10340      8.00000      0.17003        1730.

  0.52096      0.06512      8.00001      0.14352        1730.

  0.59581      0.07448      8.00000      0.15071        1730.

  0.58844      0.07356      8.00000      0.15000      NOT MAX

  0.29422      0.06620      4.44445      0.09321      NOT MAX

  0.37878      0.06620      5.72179      0.11589        1730.

  0.39410      0.06620      5.95323      0.11917        1730.

  0.39799      0.06620      6.01198      0.11991        1730.

  0.39844      0.06620      6.01879      0.11999        1730.


                 VOC CONTROL REQUIREMENT IS  32.3 PERCENT
```

APPENDIX F

EXAMPLE OF BASE-CASE ISOPLETH OUTPUT

```
***************************************
*                                     *
*  OZONE ISOPLETH PLOTTING PACKAGE    *
*     WITH OPTIONAL MECHANISMS        *
*                                     *
*          O Z I P M - 4              *
*                                     *
*            MAY, 1989                *
*                                     *
***************************************
```

```
EXAMPLE OF BASE CASE ISOPLETH


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

       TEST CITY

LATITUDE     38.629

LONGITUDE    90.206

TIME ZONE    6.0

DATE         6     21    1988

TIME         800   TO    1800     LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS     INITIAL   250.     FINAL      1700.

TIMING                START     800.     STOP       1500.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME       800     900     1000    1100    1200    1300    1400    1500

HEIGHT     250.0   503.1   821.2   1119.5  1340.2  1496.2  1610.8  1700.0


TEMPERATURE (AT THE BEGINNING OF EACH HOUR)

HOUR          0       1       2       3       4       5       6       7       8       9
             10      11

TEMP        294.0   296.0   299.0   301.0   304.0   305.0   307.0   308.0   306.0   305.0
            304.0   302.0


RELATIVE HUMIDITY (AT THE BEGINNING OF EACH HOUR)

HOUR          0       1       2       3       4       5       6       7       8       9
             10      11

RH (%)       80.0    75.0    50.0    45.0    40.0    35.0    30.0    30.0    30.0    30.0
             35.0    40.0
```

```
WATER CONCENTRATIONS (AT THE BEGINNING OF EACH HOUR)

HOUR         0       1       2       3       4       5       6       7       8       9
            10      11

PPM        19333.  20417.  16210.  16349.  17176.  15875.  15150.  15989.  14366.  13607.
           15029.  15373.

PRESSURE      29.95 INCHES OF HG


REACTIVITY

EMISSIONS       ETH  FRACTION 0.037   OLE  FRACTION 0.035   ALD2 FRACTION 0.052

EMISSIONS       FORM FRACTION 0.021   TOL  FRACTION 0.089   XYL  FRACTION 0.117

EMISSIONS       PAR  FRACTION 0.564   NR   FRACTION 0.085

ALOFT           ETH  FRACTION 0.034   OLE  FRACTION 0.020   ALD2 FRACTION 0.037

ALOFT           FORM FRACTION 0.070   TOL  FRACTION 0.042   XYL  FRACTION 0.026

ALOFT           PAR  FRACTION 0.498   NR   FRACTION 0.273

NO2/NOX       0.250
```

```
TRANSPORTED CONCENTRATIONS

ALOFT               OZONE    0.040      HYDROCARBON  0.030    NOX      0.002 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)

SPECIES     HOUR          1     2     3     4     5     6     7     8     9    10
                         11

  VOC     FRACTION     0.099 0.081 0.079 0.055 0.034 0.024 0.023 0.018 0.018 0.022
                       0.012

  NOX     FRACTION     0.215 0.163 0.149 0.109 0.073 0.050 0.051 0.042 0.038 0.047
                       0.024

  CO      FRACTION     0.038 0.056 0.041 0.034 0.034 0.034 0.034 0.038 0.041 0.045
                       0.080


TRANSPORTED BIOGENIC CONCENTRATIONS

SURFACE LAYER       ISOP     0.000       APIN         0.000

ALOFT               ISOP     0.000       APIN         0.000


THE FOLLOWING BIOGENIC SPECIES ARE TREATED AS HYDROCARBONS
(EXPRESSED AS BOND FRACTIONS)

APIN             ETH  FRACTION 0.000   OLE  FRACTION 0.500   ALD2 FRACTION 1.500
                 FORM FRACTION 0.000   TOL  FRACTION 0.000   XYL  FRACTION 0.000
                 PAR  FRACTION 0.000   NR   FRACTION 0.000


BIOGENIC EMISSIONS (IN UNITS OF PPM/HR)

SPECIES     HOUR          1     2     3     4     5     6     7     8     9    10
                         11

 ISOP                  0.000 0.000 0.000 0.000 0.001 0.001 0.002 0.002 0.001 0.001
                       0.001

 APIN                  0.000 0.000 0.000 0.000 0.001 0.001 0.002 0.001 0.001 0.001
                       0.001
                 THE FOLLOWING SIMULATIONS WERE DONE.

      NMOC          NOX          RATIO         O3

    0.00000       0.00000       0.00000     6.19867E-02

    0.00000       0.02800       0.00000     8.26974E-02

    0.00000       0.05600       0.00000     4.70933E-02

    0.00000       0.08400       0.00000     3.31751E-02

    0.00000       0.11200       0.00000     2.65932E-02

    0.00000       0.14000       0.00000     2.26974E-02

    0.00000       0.16800       0.00000     1.99119E-02

    0.00000       0.19600       0.00000     1.78783E-02

    0.00000       0.22400       0.00000     1.63376E-02

    0.00000       0.25200       0.00000     1.50636E-02

    0.00000       0.28000       0.00000     1.40032E-02

    0.20000       0.00000       0.00000     6.20564E-02

    0.20000       0.02800       7.14286     1.05297E-01

    0.20000       0.05600       3.57143     9.43855E-02

    0.20000       0.08400       2.38095     5.57804E-02

    0.20000       0.11200       1.78571     3.95178E-02

    0.20000       0.14000       1.42857     3.08421E-02

    0.20000       0.16800       1.19048     2.52848E-02

    0.20000       0.19600       1.02041     2.17718E-02

    0.20000       0.22400       0.89286     1.91602E-02

    0.20000       0.25200       0.79365     1.71695E-02

    0.20000       0.28000       0.71429     1.56914E-02

    0.40000       0.00000       0.00000     6.00081E-02

    0.40000       0.02800      14.28572     1.18297E-01

    0.40000       0.05600       7.14286     1.30707E-01

    0.40000       0.08400       4.76191     9.95114E-02
```

```
0.40000     0.11200      3.57143    6.46477E-02
0.40000     0.14000      2.85714    4.68295E-02
0.40000     0.16800      2.38095    3.61432E-02
0.40000     0.19600      2.04082    2.93161E-02
0.40000     0.22400      1.78571    2.46876E-02
0.40000     0.25200      1.58730    2.13950E-02
0.40000     0.28000      1.42857    1.89471E-02
0.60000     0.00000      0.00000    5.82304E-02
0.60000     0.02800     21.42857    1.25606E-01
0.60000     0.05600     10.71429    1.48342E-01
0.60000     0.08400      7.14286    1.47483E-01
0.60000     0.11200      5.35714    1.05377E-01
0.60000     0.14000      4.28572    7.32448E-02
0.60000     0.16800      3.57143    5.43256E-02
0.60000     0.19600      3.06122    4.25025E-02
0.60000     0.22400      2.67857    3.43116E-02
0.60000     0.25200      2.38095    2.85593E-02
0.60000     0.28000      2.14286    2.42927E-02
0.80000     0.00000      0.00000    5.69717E-02
0.80000     0.02800     28.57143    1.28725E-01
0.80000     0.05600     14.28572    1.59763E-01
0.80000     0.08400      9.52381    1.70739E-01
0.80000     0.11200      7.14286    1.57060E-01
0.80000     0.14000      5.71429    1.11763E-01
0.80000     0.16800      4.76191    8.17086E-02
0.80000     0.19600      4.08163    6.23803E-02
0.80000     0.22400      3.57143    4.90160E-02
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0.80000	0.25200	3.17460	3.95948E-02
0.80000	0.28000	2.85714	3.27368E-02
1.00000	0.00000	0.00000	5.60606E-02
1.00000	0.02800	35.71428	1.29388E-01
1.00000	0.05600	17.85713	1.66818E-01
1.00000	0.08400	11.90476	1.85116E-01
1.00000	0.11200	8.92857	1.88138E-01
1.00000	0.14000	7.14286	1.61823E-01
1.00000	0.16800	5.95238	1.18390E-01
1.00000	0.19600	5.10204	8.98018E-02
1.00000	0.22400	4.46429	7.01978E-02
1.00000	0.25200	3.96825	5.58351E-02
1.00000	0.28000	3.57143	4.52679E-02
1.20000	0.00000	0.00000	5.53239E-02
1.20000	0.02800	42.85713	1.28923E-01
1.20000	0.05600	21.42856	1.70819E-01
1.20000	0.08400	14.28571	1.94747E-01
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1.20000	0.22400	5.35714	9.76331E-02
1.20000	0.25200	4.76190	7.77631E-02
1.20000	0.28000	4.28571	6.25198E-02
1.40000	0.00000	0.00000	5.47609E-02
1.40000	0.02800	49.99998	1.27696E-01
1.40000	0.05600	24.99998	1.72843E-01
1.40000	0.08400	16.66666	2.01083E-01

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1.40000      0.14000      10.00000     2.22733E-01

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1.40000      0.19600       7.14286     1.68540E-01

1.40000      0.22400       6.25000     1.32008E-01

1.40000      0.25200       5.55555     1.05273E-01

1.40000      0.28000       5.00000     8.51101E-02

1.60000      0.00000       0.00000     5.42701E-02

1.60000      0.02800      57.14287     1.26161E-01

1.60000      0.05600      28.57143     1.73300E-01

1.60000      0.08400      19.04762     2.05178E-01

1.60000      0.11200      14.28572     2.25630E-01

1.60000      0.14000      11.42857     2.36951E-01

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1.60000      0.22400       7.14286     1.72655E-01

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1.60000      0.28000       5.71429     1.12470E-01

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1.80000      0.05600      32.14285     1.72898E-01

1.80000      0.08400      21.42857     2.07516E-01

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1.80000      0.16800      10.71429     2.53611E-01

1.80000      0.19600       9.18367     2.47534E-01

1.80000      0.22400       8.03572     2.17375E-01

1.80000      0.25200       7.14286     1.76680E-01
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   2.00000       0.02800      71.42856    1.23546E-01
   2.00000       0.05600      35.71428    1.72080E-01
   2.00000       0.08400      23.80952    2.08454E-01
   2.00000       0.11200      17.85713    2.35256E-01
   2.00000       0.14000      14.28572    2.53984E-01
   2.00000       0.16800      11.90476    2.55070E-01
   2.00000       0.19600      10.20408    2.57808E-01
   2.00000       0.22400       8.92857    2.54963E-01
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   2.00000       0.28000       7.14286    1.81379E-01
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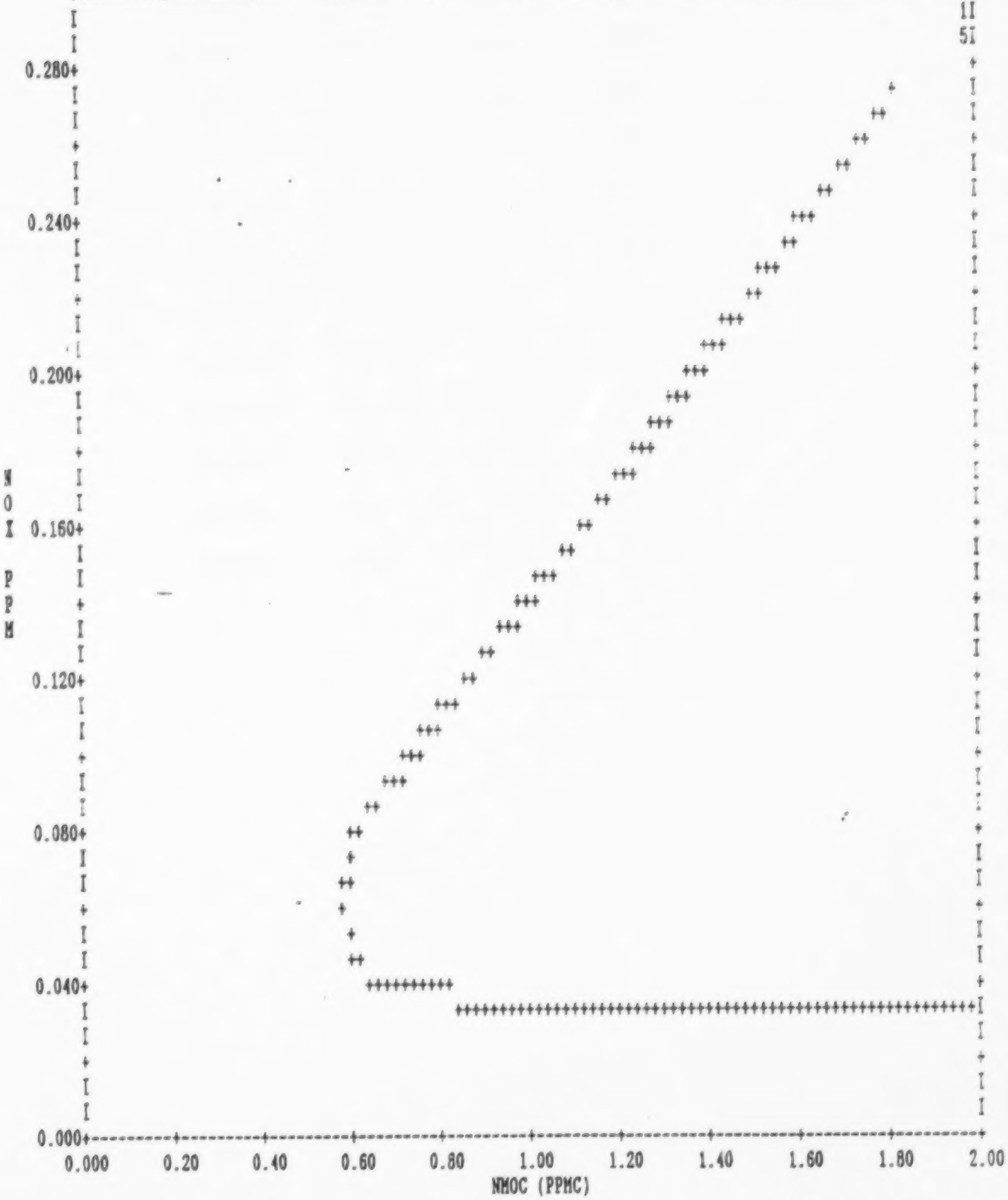
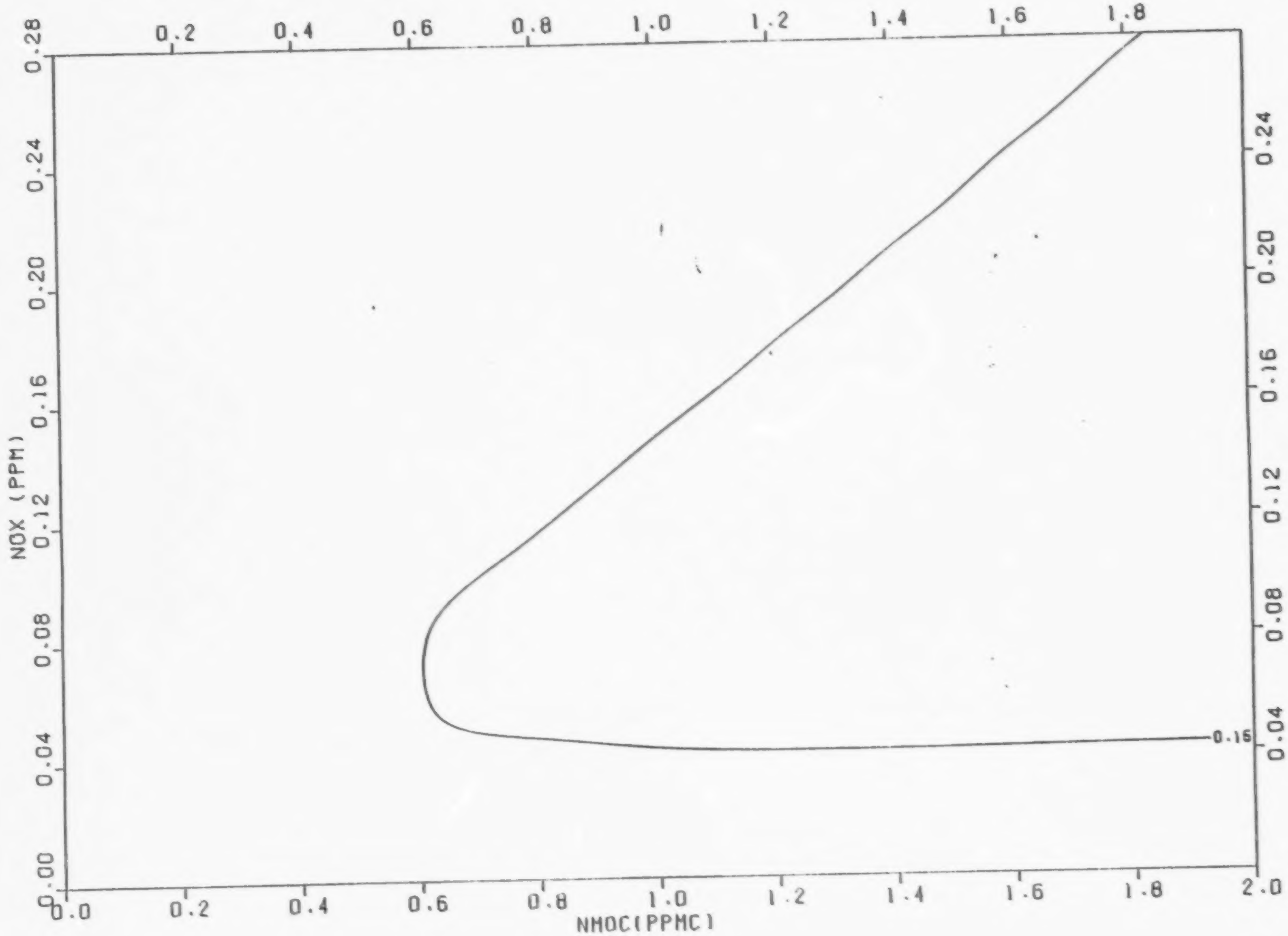


EXAMPLE OF BASE CASE ISOPLETH

THE O3 LINES ARE 0.15000



EXAMPLE OF BASE CASE ISOPLETH

APPENDIX G

EXAMPLE OF FUTURE CASE ISOPLETH OUTPUT

```
***************************************
*                                     *
*   OZONE ISOPLETH PLOTTING PACKAGE   *
*      WITH OPTIONAL MECHANISMS       *
*                                     *
*            O Z I P M - 4            *
*                                     *
*              MAY, 1989              *
*                                     *
***************************************
```

```
EXAMPLE OF FUTURE CASE ISOPLETH


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR


        TEST CITY


LATITUDE     38.629

LONGITUDE    90.206

TIME ZONE    6.0

DATE         6     21    1988

TIME         800   TO    1800     LOCAL DAYLIGHT TIME



DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS      INITIAL   250.     FINAL       1700.

TIMING                 START     800.     STOP        1500.



MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME       800     900     1000     1100     1200     1300     1400     1500

HEIGHT     250.0   503.1   821.2   1119.5   1340.2   1496.2   1610.8   1700.0



TEMPERATURE (AT THE BEGINNING OF EACH HOUR)

HOUR           0       1       2       3       4       5       6       7       8       9
              10      11

TEMP       294.0   296.0   299.0   301.0   304.0   305.0   307.0   308.0   306.0   305.0
           304.0   302.0



RELATIVE HUMIDITY (AT THE BEGINNING OF EACH HOUR)

HOUR           0       1       2       3       4       5       6       7       8       9
              10      11

RH (%)      80.0    75.0    50.0    45.0    40.0    35.0    30.0    30.0    30.0    30.0
            35.0    40.0
```

```
WATER CONCENTRATIONS (AT THE BEGINNING OF EACH HOUR)

HOUR          0       1       2       3       4       5       6       7       8       9
             10      11

PPM       19333.  20417.  16210.  16349.  17176.  15875.  15159.  15989.  14366.  13607.
          15029.  15373.

PRESSURE      29.95 INCHES OF HG


REACTIVITY

EMISSIONS        ETH  FRACTION 0.037   OLE  FRACTION 0.035   ALD2 FRACTION 0.052

EMISSIONS        FORM FRACTION 0.021   TOL  FRACTION 0.089   XYL  FRACTION 0.117

EMISSIONS        PAR  FRACTION 0.564   NR   FRACTION 0.085

ALOFT            ETH  FRACTION 0.034   OLE  FRACTION 0.020   ALD2 FRACTION 0.037

ALOFT            FORM FRACTION 0.070   TOL  FRACTION 0.042   XYL  FRACTION 0.026

ALOFT            PAR  FRACTION 0.498   NR   FRACTION 0.273

NO2/NOX      0.250
```

```
TRANSPORTED CONCENTRATIONS

ALOFT               OZONE    0.040     HYDROCARBON  0.024    NOX     0.002 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)

SPECIES     HOUR           1     2     3     4     5     6     7     8     9    10
                          11

  VOC      FRACTION     0.099 0.081 0.079 0.055 0.034 0.024 0.023 0.018 0.018 0.022
                        0.012

  NOX      FRACTION     0.215 0.163 0.149 0.109 0.073 0.050 0.051 0.042 0.038 0.047
                        0.024

  CO       FRACTION     0.019 0.028 0.021 0.017 0.017 0.017 0.017 0.019 0.021 0.023
                        0.030


TRANSPORTED BIOGENIC CONCENTRATIONS

SURFACE LAYER        ISOP     0.000      APIN         0.000

ALOFT                ISOP     0.000      APIN         0.000


THE FOLLOWING BIOGENIC SPECIES ARE TREATED AS HYDROCARBONS
(EXPRESSED AS BOND FRACTIONS)

APIN            ETH  FRACTION 0.000   OLE  FRACTION 0.500   ALD2 FRACTION 1.500
                FORM FRACTION 0.000   TOL  FRACTION 0.000   XYL  FRACTION 0.000
                PAR  FRACTION 6.000   NR   FRACTION 0.000


BIOGENIC EMISSIONS (IN UNITS OF PPM/HR)

SPECIES     HOUR           1     2     3     4     5     6     7     8     9    10
                          11

  ISOP                  0.000 0.000 0.000 0.000 0.001 0.001 0.002 0.002 0.001 0.001
                        0.001

  APIN                  0.000 0.000 0.000 0.000 0.001 0.001 0.002 0.001 0.001 0.001
                        0.001
```

```
                    THE FOLLOWING SIMULATIONS WERE DONE.

       NMOC          NOX           RATIO          O3

     0.00000       0.00000        0.00000     6.14826E-02

     0.00000       0.02800        0.00000     7.31059E-02

     0.00000       0.05600        0.00000     4.40069E-02

     0.00000       0.08400        0.00000     3.16574E-02

     0.00000       0.11200        0.00000     2.57113E-02

     0.00000       0.14000        0.00000     2.20918E-02

     0.00000       0.16800        0.00000     1.95288E-02

     0.00000       0.19600        0.00000     1.76081E-02

     0.00000       0.22400        0.00000     1.61134E-02

     0.00000       0.25200        0.00000     1.48988E-02

     0.00000       0.28000        0.00000     1.38806E-02

     0.20000       0.00000        0.00000     6.19389E-02

     0.20000       0.02800        7.14286     1.03811E-01

     0.20000       0.05600        3.57143     8.86761E-02

     0.20000       0.08400        2.38095     5.28854E-02

     0.20000       0.11200        1.78571     3.76923E-02

     0.20000       0.14000        1.42857     2.96138E-02

     0.20000       0.16800        1.19048     2.45393E-02

     0.20000       0.19600        1.02041     2.11628E-02

     0.20000       0.22400        0.89286     1.87226E-02

     0.20000       0.25200        0.79365     1.68443E-02

     0.20000       0.28000        0.71429     1.54300E-02

     0.40000       0.00000        0.00000     5.98908E-02

     0.40000       0.02800       14.28572     1.17304E-01

     0.40000       0.05600        7.14286     1.28274E-01
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0.40000      0.08400       4.76191    9.42453E-02
0.40000      0.11200       3.57143    6.14254E-02
0.40000      0.14000       2.85714    4.47667E-02
0.40000      0.16800       2.38095    3.47616E-02
0.40000      0.19600       2.04082    2.82650E-02
0.40000      0.22400       1.78571    2.39419E-02
0.40000      0.25200       1.58730    2.08009E-02
0.40000      0.28000       1.42857    1.84733E-02
0.60000      0.00000       0.00000    5.32385E-02
0.60000      0.02800      21.42857    1.24823E-01
0.60000      0.05600      10.71429    1.46950E-01
0.60000      0.08400       7.14286    1.44034E-01
0.60000      0.11200       5.35714    1.00593E-01
0.60000      0.14000       4.28572    6.99520E-02
0.60000      0.16800       3.57143    5.23176E-02
0.60000      0.19600       3.06122    4.06481E-02
0.60000      0.22400       2.67857    3.28991E-02
0.60000      0.25200       2.38095    2.76108E-02
0.60000      0.28000       2.14286    2.35838E-02
0.80000      0.00000       0.00000    5.69435E-02
0.80000      0.02800      28.57143    1.28389E-01
0.80000      0.05600      14.28572    1.58729E-01
0.80000      0.08400       9.52381    1.58927E-01
0.80000      0.11200       7.14286    1.52706E-01
0.80000      0.14000       5.71429    1.07549E-01
0.80000      0.16800       4.76191    7.86303E-02
0.80000      0.19600       4.08163    6.00352E-02
0.80000      0.22400       3.57143    4.71128E-02
0.80000      0.25200       3.17460    3.84468E-02
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0.80000	0.28000	2.85714	3.19004E-02
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1.00000	0.02800	35.71428	1.29246E-01
1.00000	0.05600	17.85713	1.66015E-01
1.00000	0.08400	11.90476	1.83798E-01
1.00000	0.11200	8.92857	1.85734E-01
1.00000	0.14000	7.14286	1.56784E-01
1.00000	0.16800	5.95238	1.14490E-01
1.00000	0.19600	5.10204	8.64215E-02
1.00000	0.22400	4.46429	6.76017E-02
1.00000	0.25200	3.96825	5.41054E-02
1.00000	0.28000	3.57143	4.41031E-02
1.20000	0.00000	0.00000	5.52917E-02
1.20000	0.02800	42.85713	1.28685E-01
1.20000	0.05600	21.42856	1.70359E-01
1.20000	0.08400	14.28571	1.93758E-01
1.20000	0.11200	10.71428	2.04307E-01
1.20000	0.14000	8.57143	1.98262E-01
1.20000	0.16800	7.14286	1.59938E-01
1.20000	0.19600	6.12245	1.21334E-01
1.20000	0.22400	5.35714	9.46140E-02
1.20000	0.25200	4.76190	7.52475E-02
1.20000	0.28000	4.28571	6.08634E-02
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1.40000	0.02800	49.99998	1.27625E-01
1.40000	0.05600	24.99998	1.72426E-01
1.40000	0.08400	16.66666	2.00360E-01
1.40000	0.11200	12.50000	2.16305E-01
1.40000	0.14000	10.00000	2.20914E-01

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1.40000     0.16800      8.33333    2.05908E-01
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1.40000     0.22400      6.25000    1.28258E-01
1.40000     0.25200      5.55555    1.02268E-01
1.40000     0.28000      5.00000    8.26709E-02
1.60000     0.00000      0.00000    5.42542E-02
1.60000     0.02800     57.14287    1.26089E-01
1.60000     0.05600     28.57143    1.73061E-01
1.60000     0.08400     19.04762    2.04639E-01
1.60000     0.11200     14.28572    2.24847E-01
1.60000     0.14000     11.42857    2.35486E-01
1.60000     0.16800      9.52381    2.34466E-01
1.60000     0.19600      8.16327    2.10096E-01
1.60000     0.22400      7.14286    1.68030E-01
1.60000     0.25200      6.34921    1.34772E-01
1.60000     0.28000      5.71429    1.09242E-01
1.80000     0.00000      0.00000    5.38059E-02
1.80000     0.02800     64.28571    1.24695E-01
1.80000     0.05600     32.14285    1.72718E-01
1.80000     0.08400     21.42857    2.07099E-01
1.80000     0.11200     16.07143    2.30721E-01
1.80000     0.14000     12.85715    2.45648E-01
1.80000     0.16800     10.71429    2.51889E-01
1.80000     0.19600      9.18367    2.44592E-01
1.80000     0.22400      8.03572    2.12557E-01
1.80000     0.25200      7.14286    1.72810E-01
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2.00000     0.00000      0.00000    5.34195E-02
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2.00000      0.02800      71.42856     1.23649E-01

2.00000      0.05600      35.71428     1.71864E-01

2.00000      0.08400      23.80952     2.08105E-01

2.00000      0.11200      17.85713     2.34744E-01

2.00000      0.14000      14.28572     2.53122E-01

2.00000      0.16800      11.90476     2.64125E-01

2.00000      0.19600      10.20408     2.66015E-01

2.00000      0.22400       8.92857     2.51539E-01

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2.00000      0.28000       7.14286     1.77986E-01
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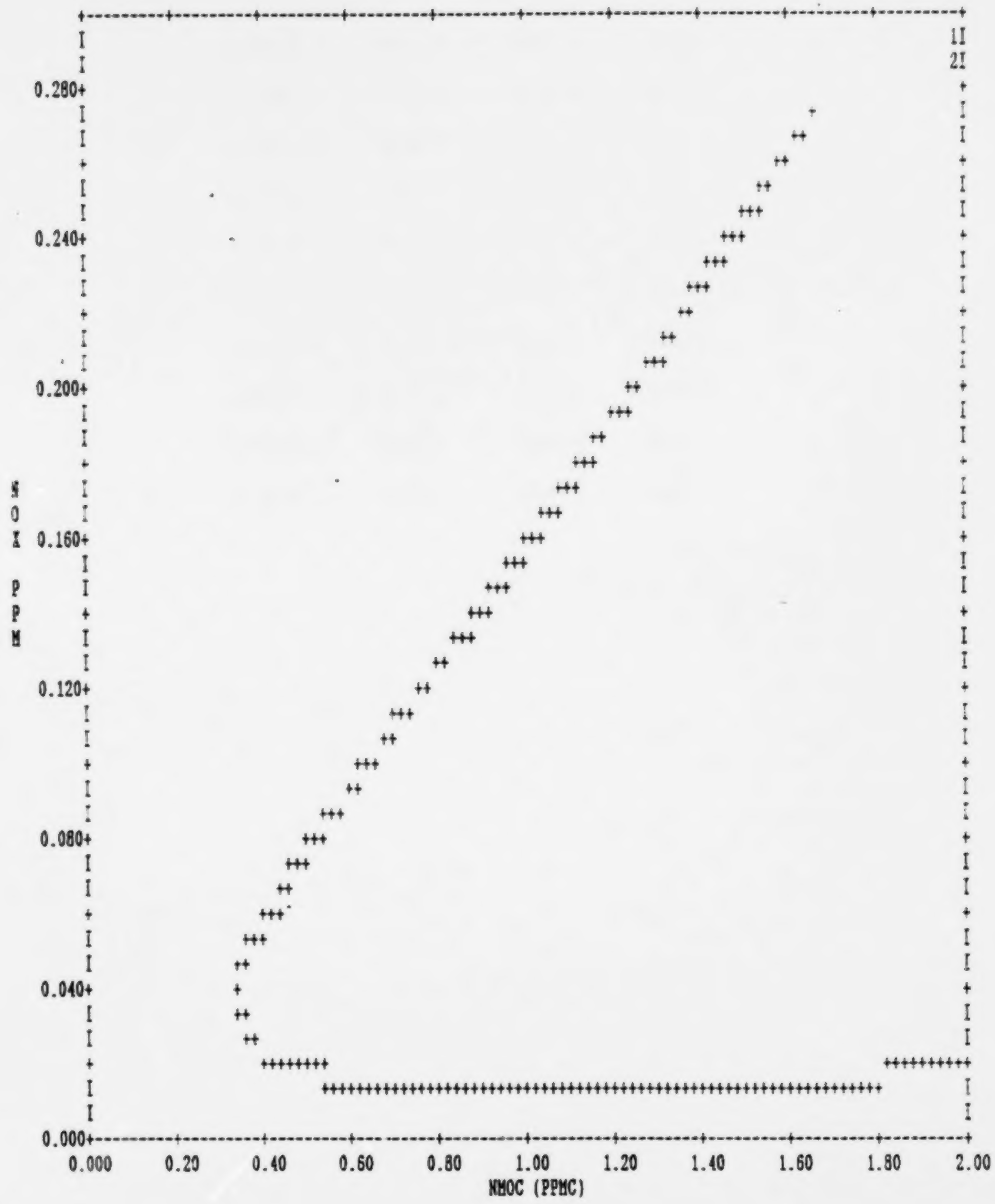
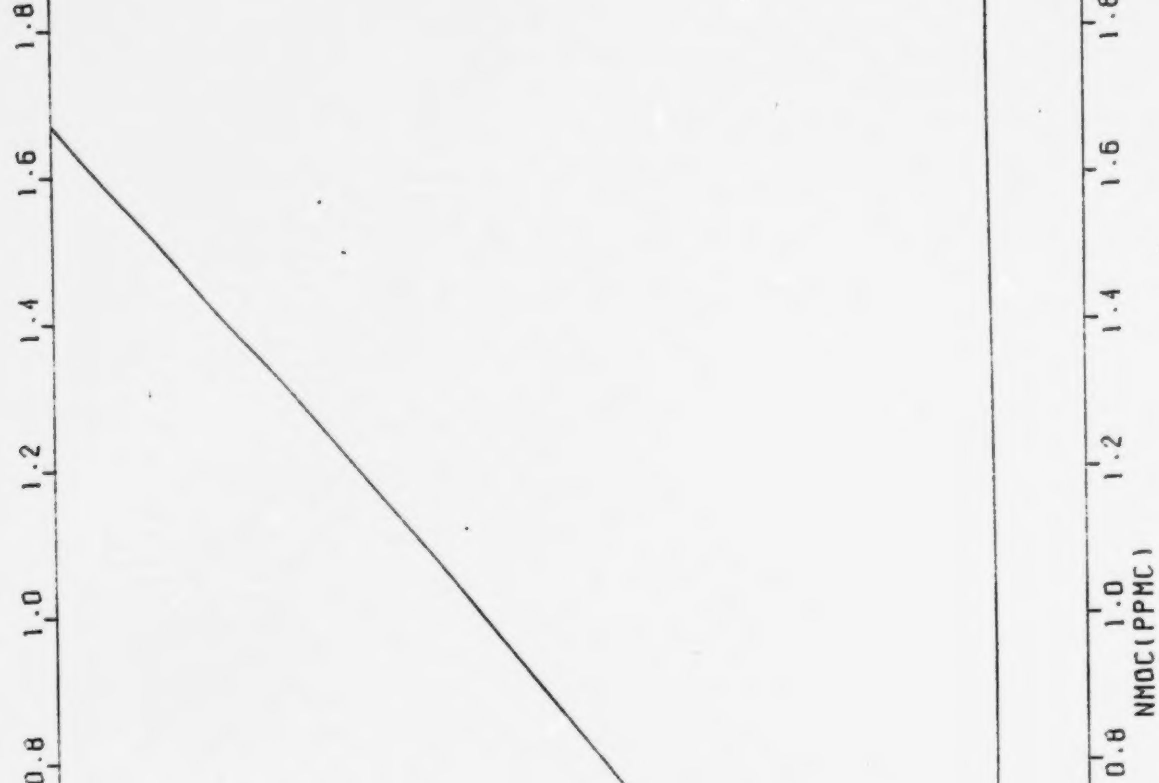


EXAMPLE OF FUTURE CASE ISOPLETH

THE 03 LINES ARE 0.12000



EXAMPLE OF FUTURE CASE ISOPLETH